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FURTHER STUDIES OF PARAMETERIZED AIR QUALITY MODELING METHODS FOR MATERIALS DAMAGE ASSESSMENT

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16. ABSTRACT

Damage to materials is one of the concerns of the National Acid Precipitation Assessment Program (NAPAP). This project addressed the concern by providing an inexpensive method for estimating the deposition of hydrogen ions and sulfur dioxide on spatial scales compatible with materials distributions within urban areas. Since monitoring data are taken at only a few discrete points within any urban area the direct use of such data was rejected as unsuitable for meeting the concern.

Comparison of output from the Parameterized Air Quality Model Annual (PAQMAN) developed earlier in this project shows that the model values are generally within a factor of two of the observations. The model is sensitive to the size of the emissions grid cells especially in the 1 to 2 km size range.

The most suitable use for PAQMAN is as a rapid screening technique for examining the effect of thousands of point sources of sulfur dioxide across an extensive region. Some of the automated procedures developed for PAQMAN have wider application.

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ABSTRACT

One of the components of the National Acid Precipitation Assessment Program (NAPAP) deals with damage to materials in the environment. Such an assessment requires detailed information on deposition of corrosive agents, namely SO_2 and wet H^+, on spatial scales compatible with materials distributions in urban areas. The objective was to provide sufficiently accurate deposition estimates for materials damage for over 100 cities, within very limited time and cost constraints.

Since extant urban SO_2 monitoring data are inadequate to characterize the distribution of air quality within cities (i.e., monitors tend to be located only to meet specific regulatory needs), a modeling approach was necessary to estimate detailed annual average SO_2 concentrations. The basic approach used was one of parameterization, in which closed-form algorithms are developed for point and area sources which mimic the performance of EPA's Climatological Dispersion Model (CDM), and allow rapid assessment of a large number of sources. The modeling system, called PAQMAN (Parameterized Air Quality Model ANnual), was successfully applied to over 100 urban areas in the Northeastern U.S. in which materials distributions have been derived.

Sensitivity analyses of various model components and assumptions were performed and are described in this report. The results indicate that model calculations are most sensitive to emission grid cell size (particularly 1-2 km) and to the treatment of a given source as an area or point source depending on stack height. Comparisons between CDM and PAQMAN calculations show PAQMAN to overpredict or under-predict point source impacts for individual MSA's, suggesting that wind direction effects should be accounted for in lieu of directional averaging. The parameterized approach developed for point sources using the McElroy-Pooler dispersion coefficients are supported by the use of the Brigg's curves as well. Comparisons between PAQMAN values and observed data (grid square averages) for several major cities indicate acceptable agreement, generally within a factor of 2.

When considering aggregated effects across an extensive region involving thousands of sources, PAQMAN is a very suitable tool for estimating SO_2 distributions in urban areas. Its automated source-receptor allocation procedures allow for the rapid assessment of impacts for many sources and receptors with minimal user-imput requirements and computer running times. Should the scope of future accessments focus on a more detailed study of a single city or a few cities, more in-depth models may be more suitable. Nevertheless, some of the automated procedures developed in PAQMAN would be useful in alternative models as well.

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1.0 INTRODUCTION

Assessment of damage to materials in the built environment is one of the components of the National Acid Precipitation Assessment Program (NAPAP). Such damage can result from both dry and wet deposition of corrosive agents in the atmosphere, and therefore such assessments require appropriate air quality and deposition estimates. One of the benefits of reduced acid deposition could thus be longer lifetimes of various structures containing sensitive materials. With respect to common construction materials, as opposed to outdoor works of art, such benefits are primarily of interest in aggregated economic terms, i.e., annualized dollar savings for a city, state, or region. For example, some previous estimates were made for 117 metropolitan statistical areas in the 17 Northeastern states.[1]

1.1 Modeling Requirements

Estimates of economic benefits are usually made by comparing annual maintenance and repair expenditures under current environmental conditions with those projected to occur after some acidic deposition control strategy has been imposed. Current conditions could be estimated either from extant monitoring data or by use of mathematical models; mathematical models are required to evaluate a priori the potential benefits of candidate control strategies.

For assessment purposes, the linkages between damage to specific materials and the presence of various corrosive agents in the atmosphere are made by using mathematical damage functions which have been derived from field and laboratory tests. The atmospheric species of interest for materials damage due to acidic deposition include SO_2, HNO_3, particulates, and wet deposition of H^+; photochemical oxidants and organic acids may also be of interest under some circumstances. However, currently available test results have limited present damage functions to (gaseous) SO_2 and wet deposition of acidity $(H^+)^2$. This report is concerned with methods of estimating annual average concentration levels of SO_2 in urban areas, to be used in conjunction with such damage functions in deriving aggregate economic estimates for large metropolitan areas. It describes work performed subsequent to the development of the original PAQMAN* modeling system.[3]

1.2 Modeling Resolution Requirements

An accurate economic assessment of materials damage requires the evaluation of the following integral (Eq. 1) over a time period long enough to include actual maintenance and replacements of the materials at risk, with the summations performed over the geographic area, building components and materials of interest, and pollutants that might be affected by controls. Comparison of the integration results for various control scenarios yields the desired cost benefit data.

*Parameterized Air Quality Model ANnual.

$$\text{Damage } \$ = \sum_{ijkm} \int_{t1}^{t2} \left(P_{ijt} \cdot DF_{ikm} \cdot I_{jkmt} \cdot E_{km} \right) dt \qquad (1)$$

where

P = pollutants (ijt)
DF = damage function (ikm)
I = materials inventory (jkmt)
E = economic function (km)

with indices

i, pollutant species;
j, space (geographic location);
k, building component;
m, material type;
t, time.

Obviously, if all the data elements (P and I) were randomly distributed in space (j) without interactions, then the assessment could be based on the overall averages for each constituent. However, in reality, the types of materials (I) found in cities are related to environmental factors (P) and thus are not independent; it is reasonable to expect different materials to be used in industrial (high SO_2) sections of a city than in residential (lower SO_2) areas, for example.

Thus the choice of spatial integration step (j) depends on the homogeneity of both the environment and of the distribution of materials. Such spatial material distributions may be derived from Census tract data, for example. In this instance, no detail is available within the census tract, and thus this geographic unit would define the required degree of resolution of the assessment. Census tracts range in size from about 1 to hundreds of square kilometers.

The spatial resolution of environmental data is generally much coarser. Typical large metropolitan areas may have only a few monitoring stations. Up until the mid 1970's New York City had one of the densest SO_2 networks with 40 stations, resulting in a density of about 1 in 20 km^2. Current networks are generally much less dense. In theory, model calculations may be made on any scale of resolution desired. However, emissions source locations are often not given at less than 1-km resolution (in addition, space heating emissions are often derived from census tract data), and thus would be limited as described above for the materials distribution. As the computing grid scale decreases, precision may increase, but the number of points considered and thus computing times will increase with the square of linear dimensions.

Previous economic estimates were based on SO_2 estimates resolved to 5x5 km grid square averages, using the PAQMAN modeling algorithms. This grid size was selected as a compromise between precision and computing time requirements. The modeling concepts used to derive the PAQMAN modeling system are described below in Section 2. Additional studies which have been performed to examine the sensitivity of some of the modeling concepts are addressed in Section 3.

2.0 THE PAQMAN MODELING SYSTEM

The PAQMAN system is a parameterized scheme in which simplified algorithms describing the dispersion of both point and area sources were developed, intended to emulate EPA's Climatological Dispersion Model (CDM)[4]. This system was used to provide annual average SO_2 concentration estimates over 5-km grids encompassing an MSA*, and was derived to allow the expedient assessment of the impacts of many sources and receptors in an urban area, with minimal computer storage and user input requirements.

2.1 CDM Specifications

The parametric studies used to develop the PAQMAN algorithm based on EPA's CDM model involved a range of stack heights and flue gas exit conditions for point sources; various geometric patterns and emission densitites were used for area sources. Following the recommendations of EPA for urban areas[5], the McElroy-Pooler dispersion coefficients were used for point sources while the Pasquill-Gifford (P-G) coefficients were applied to area sources. Plume rise was calculated according to Briggs[6]. Removal processes were described by a constant exponential decay; a 3-hour half life was used. Three wind roses were used for the parametric studies: New York (JFK), Pittsburgh (PIT) and Cincinnati (CVG). These were then combined into two generic categories: "coastal" (New York) and "interior" (a blend of Pittsburgh and Cincinnati), in order to eliminate site-specific wind roses in favor of regionally representative meteorology.

2.2 Point Source Algorithms

The point source calculation algorithms were based on the use of the avcraged distance (r_{max}) from the source to the location of the maximum annual average ground-level concentration as a scaling parameter. This distance was found to be proportional to stack height as shown in Figure 1. The downwind ratio of concentration with respect to the maximum concentration was found to be a function of the ratio of downwind distance to this scale length, r_{max} (Figure 2). The maximum ground-level concentration (χ/Q) was an inverse-squared function of stack height as shown in Figure 3. Such a parameterization scheme combines all stack heights into one generalized representation, and implicitly averages all wind directions. Figure 4 depicts the results of combining stack heights in this fashion. As shown, the total spread among various stack heights reaches a factor of about 2 at a concentration ratio of 0.01, at which point absolute SO_2 levels will be quite small and the error unimportant. By averaging the concentrations at a given downwind distance for all directions, a real isopleth pattern is averaged into essentially a circular one. This simplification results in requiring only the source-receptor separation distance to estimate the annual average impact, a major computational simplification.

These simplifying assumptions and methods limit the application of the parameterized model to cases where there are many point sources of varying heights and locations. In such instances, the errors incurred from one source tend to be cancelled by the others, reducing any net bias that might be introduced. The methodology is also limited to estimating annual average SO_2 levels since wind direction is neglected.

* MSA: Metropolitan Statistical Area

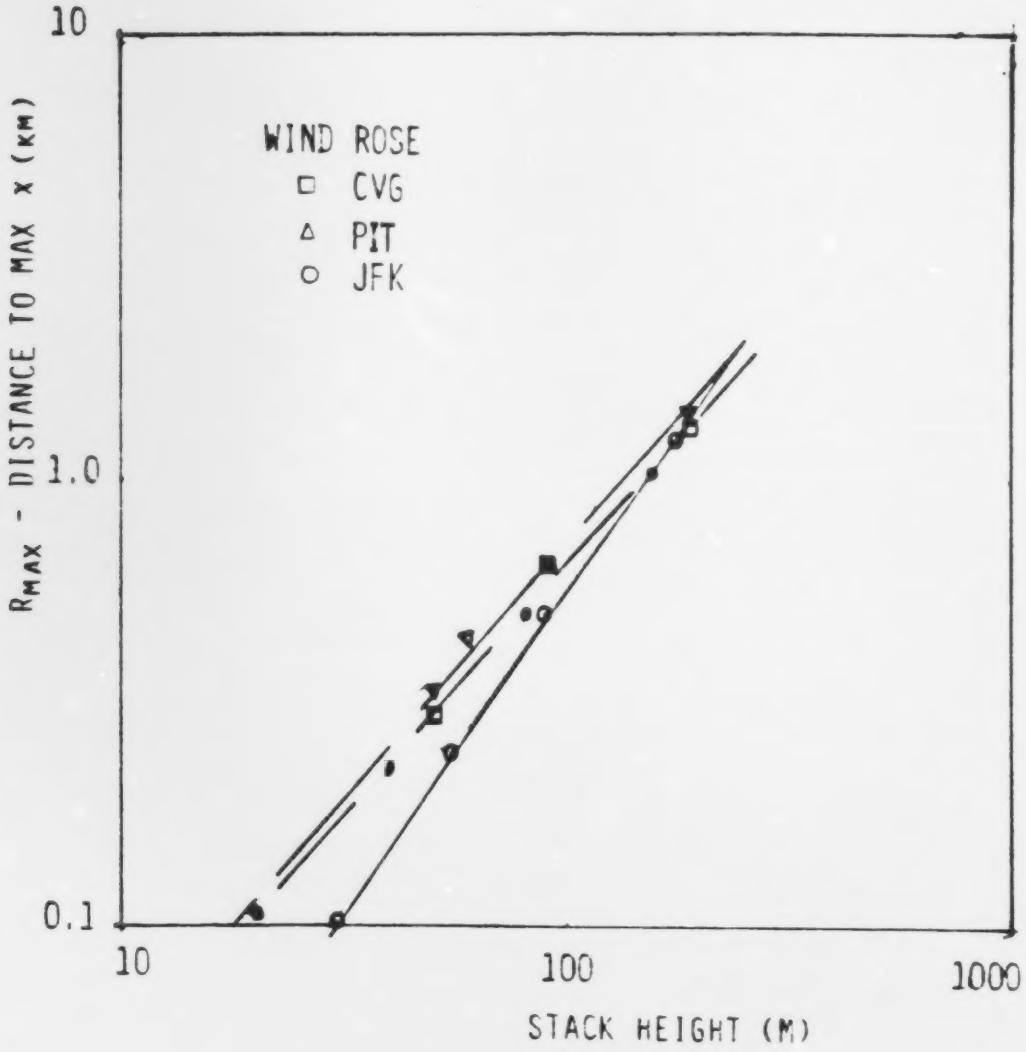


Figure 1. Downwind Distance to Maximum Concentration
CDM Model
McElroy-Pooler σ's

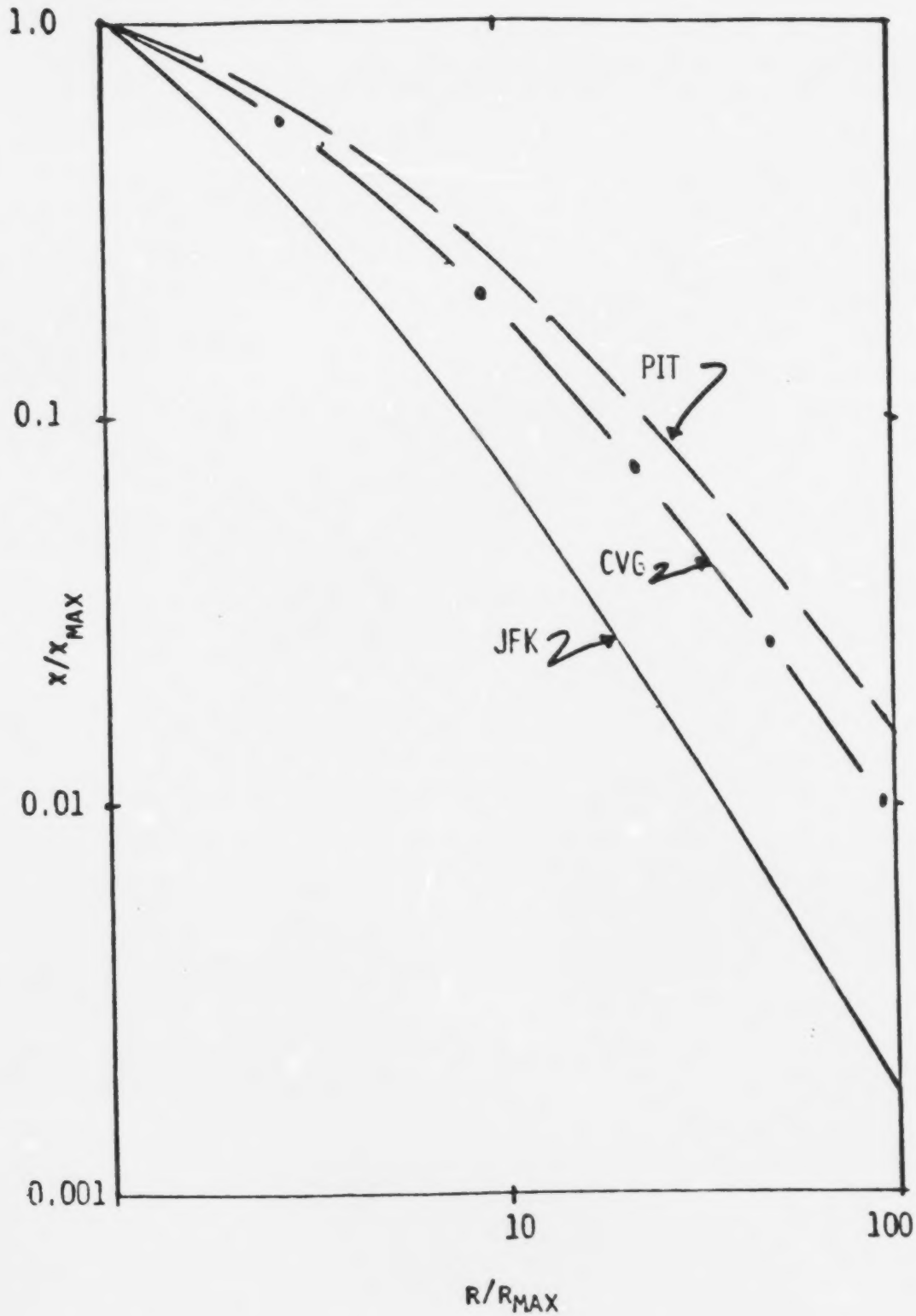


Figure 2. Concentration Ratio vs. Distance Ratio
CDM Model
McElroy-Pooler σ's

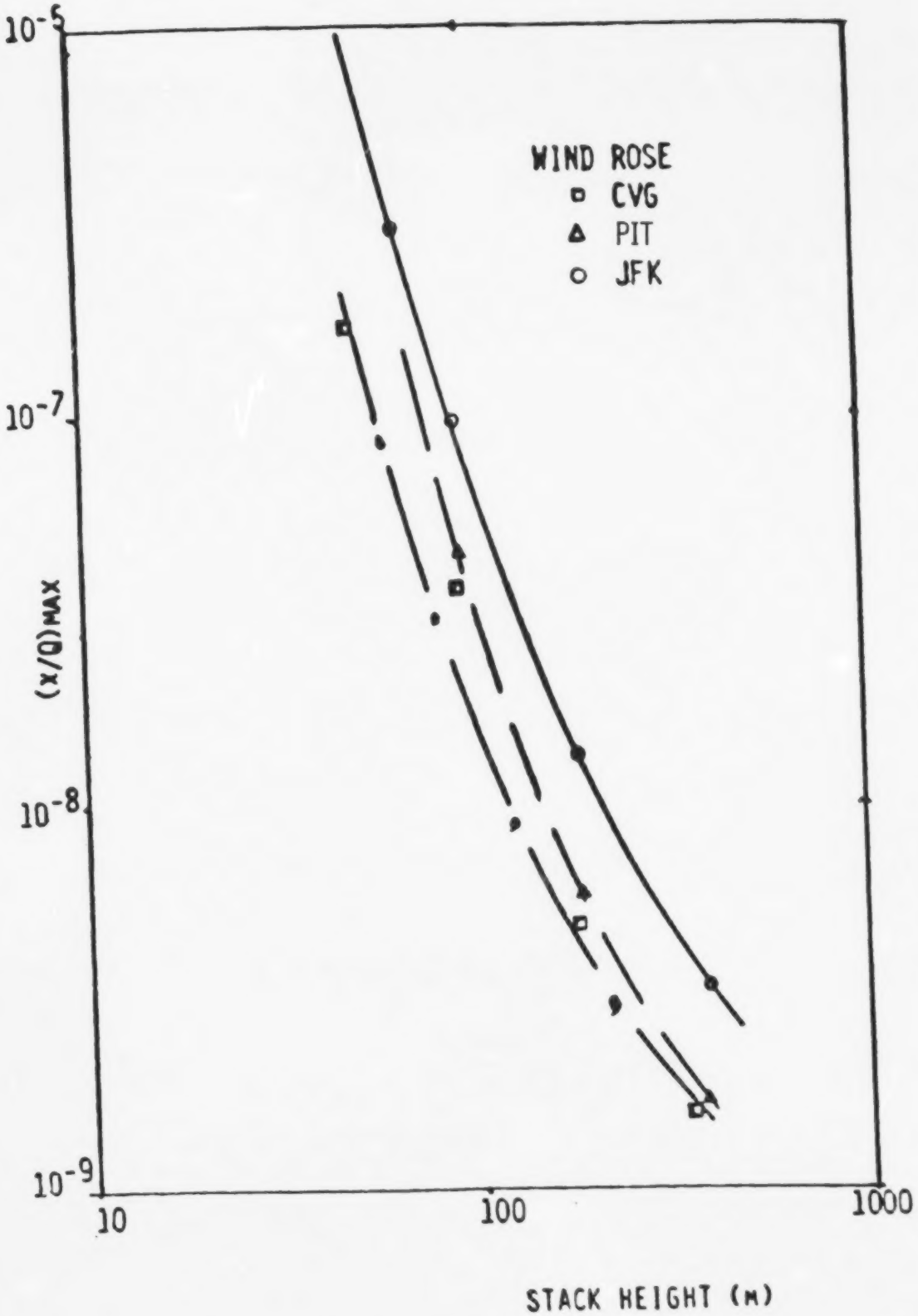


Figure 3. Max. Concentration vs. Stack Height
CDM Model
McElroy-Pooler σ's

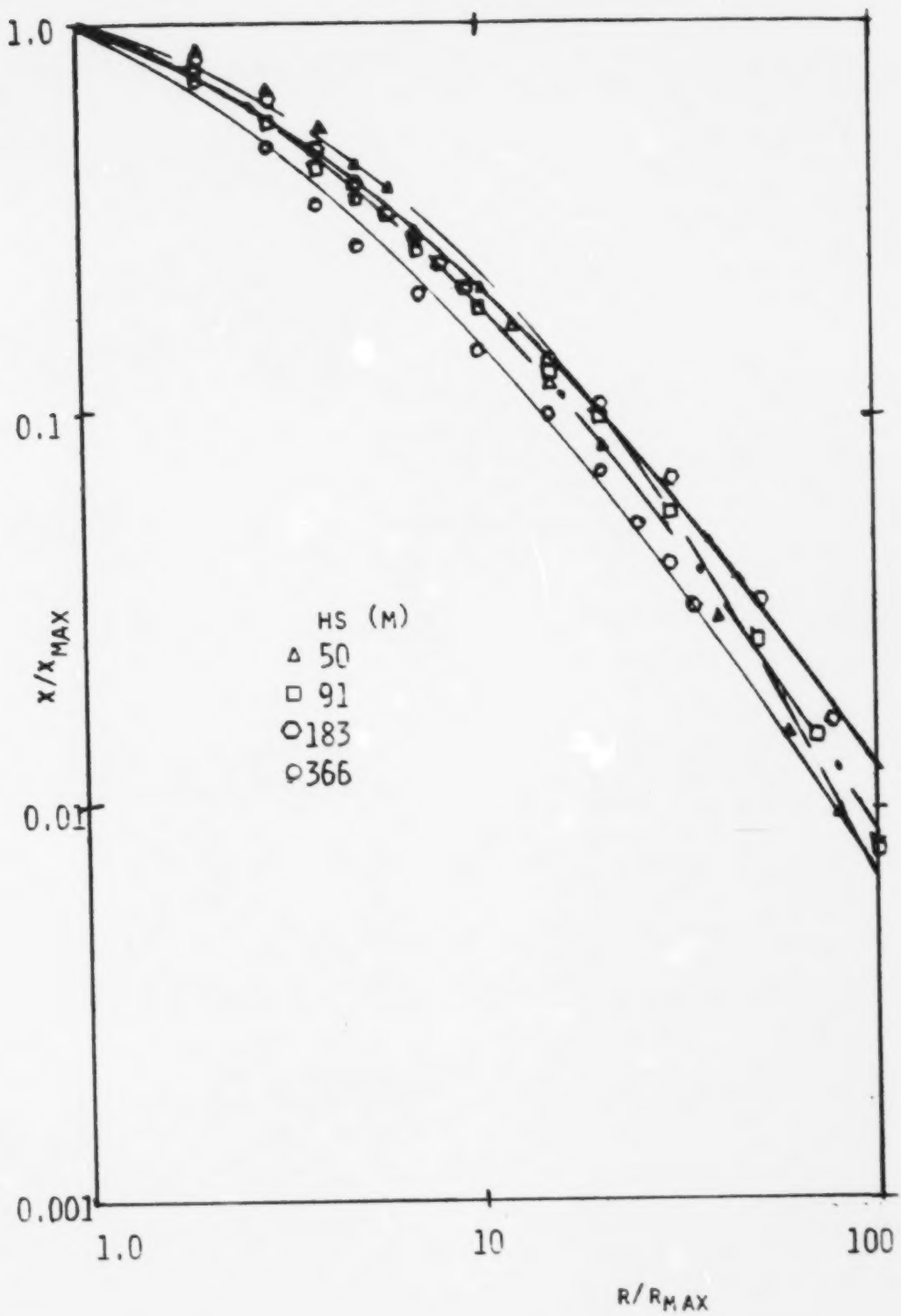


Figure 4. Concentration Ratio vs. Distance Ratio
CVG Wind Rose - Varying H_s
McElroy-Pooler c's.

2.3 Area Source Algorithms

Emission density (Q/A) and scale length (grid size) were the controlling parameters for the area source calculation algorithm (Figure 5). The underlying assumption is that concentration patterns tend to "flow" from areas of high emission density into adjacent areas of lower emission density, but not vice-versa. This was deduced from parametric calculations with CDM using concentric square source regions of varying emission densities.

2.4 Model Source Allocation Algorithms

A rectangular grid (5-km spacing) was overlaid encompassing the census tract centroids within each MSA. All sources inside this grid were included in the model calculations. Sources with stack heights less than or equal to 200 ft. were grouped and treated as area sources; those with stack heights greater than 200 ft. were treated as point sources in the model (see Section 3.2). Sources within 50 km outside of the grid boundaries were all treated as point sources, but were retained only if their concentration at the nearest grid cell centroid exceeded 0.1 $\mu g/m^3$. This procedure was very effective in eliminating unnecessary calculations, which reduced computer time substantially. In addition, the emissions from groups of sources located within 0.1 km of each other were aggregated, and a weighted average stack height was used in the calculation algorithms. While this may tend to overestimate the combined concentration if the stack heights in the groups differ greatly, it prevents groups of small sources from being overlooked because each is too small to meet the 0.1-$\mu g/m^3$ criterion.

Source emissions data were obtained from the NAPAP emissions inventory (Version 2.0) for 1980, which contains about 40,000 point sources. Background SO_2 estimates (due to sources >50 km from the MSA boundary) were supplied by exogenous calculations based on Shannon's ASTRAP Model.[7]

2.5 Model Attributes for Materials Damage Assessment

The major attribute of PAQMAN is its ability to rapidly assess the impacts of a large number of sources and receptors. The automated features of its design, outlined in Table 1, eliminate extensive input requirements on the part of the user relative to "conventional" models such as CDM, and significantly reduces computing times as shown in Table 2. This may not be so important when a single city is considered, but is considerable when the impacts of thousands of sources for many areas are involved, which was the rationale for the development of the PAQMAN modeling system. An example of the computer coding needed to access the system is provided in Table 3.

While the simplified calculation methods may produce individual errors (i.e., over- or underprediction of a given source impact), the interest in the materials damage assessment is in the spatially integrated effects across all MSA's. Such errors tend to become smoothed out when averaged over a given MSA (Figure 6 shows agreement between MSA-averaged PAQMAN and MSA-averaged observed SO_2 values within a factor of 2), and will be further damped when averaged over many MSA's.

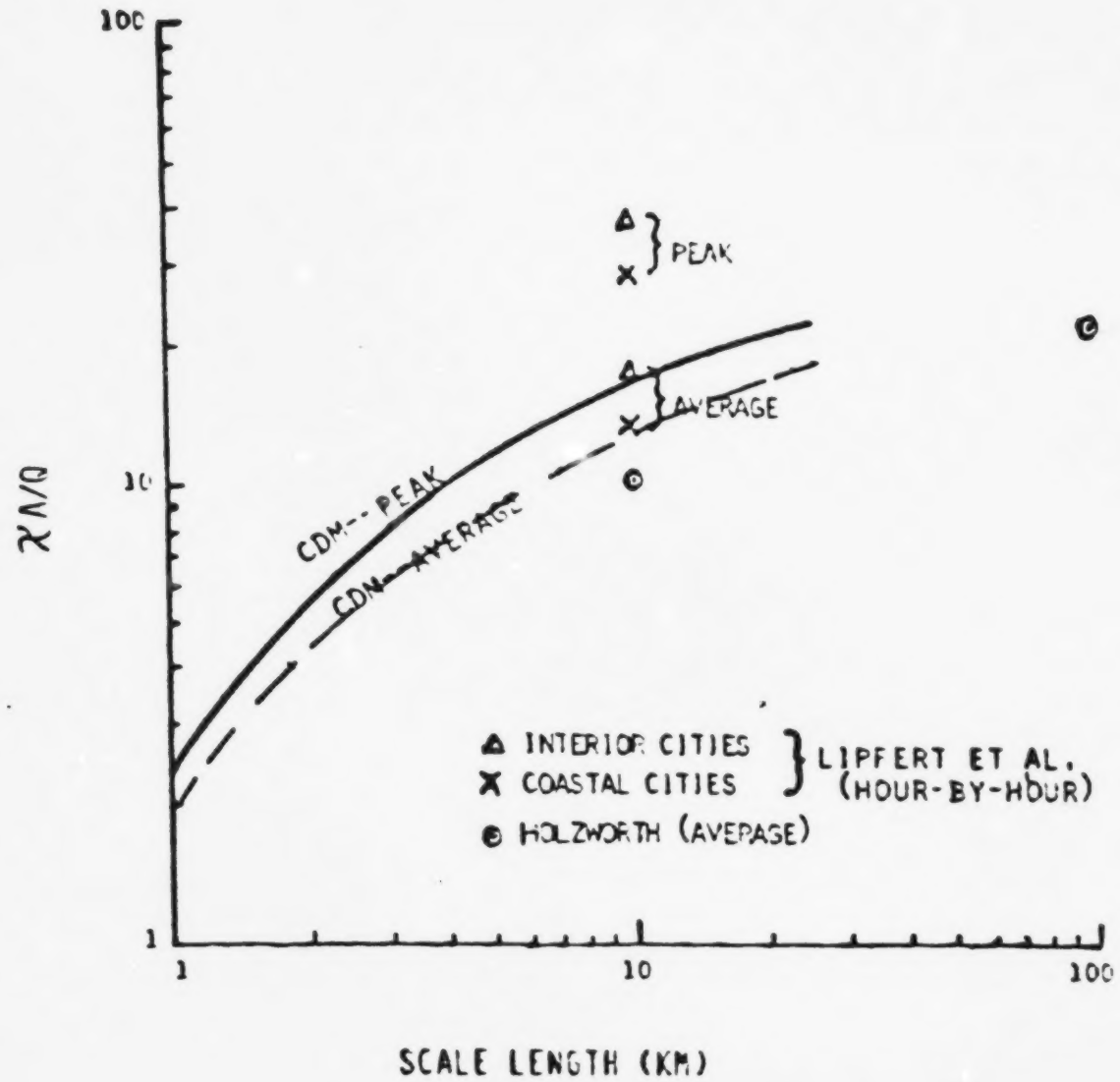


Figure 5. Scale Effect on Area-Source Diffusion (Various Models and Wind Roses)

Table 1

CDM vs. - PAQMAN MODEL INPUT REQUIREMENTS

	CDM	PAQMAN
METEOROLOGY	Star - stability wind rose (Joint frequency distribution of wind speed, wind direction and stability).	Location designator (coastal or interior Site)
SOURCES	• Assignment of each source as point or area source	Sources selected from master inventory file. Location with respect to receptor grid and assignment as area/point source performed automatically using latitude -longitude coordinates.
	• Individual source parameters (Q_s, H_s, V_s, T_s, D_s)	
	• Manual aggregation of area sources - development of emission grids, particularly if variable-size emission grids are used.	Area sources automatically aggregated to 5-km emission grids.
RECEPTORS	Develop receptor grid	5-km grid produced internally which overlaps each MSA*.

* Metropolitan Statistical Area

Table 2

CDM - vs. PAQMAN COMPUTING TIMES FOR A TYPICAL MSA

	GRID SPACING		COMPUTING TIME	
			VAX 11-730	CDC 6600
CDM	50 x 33 1-km	Receptor Grid Emission Grids	5 Days	6 Hours
CDM	11 x 7 5-km	Receptor Grid Emission Grids	40 Minutes	2 Minutes
PAQMAN	11 x 7 5-km	Receptor Grid Emission Grids	5 Minutes	15 Seconds

Table 3

EXAMPLE OF PAQMAN EXECUTION CODE AND VARIABLE INPUT DESCRIPTIONS

Execution Code

Column 1

```
RUN PAQMAN.EXE
INTERIORW
3280
1170        MSA Codes
5440
0000        (end of MSA indicator)
```

Variable Input Description

Variable Description	Format	Example
Meteorology Flag*	---	COASTAL
MSA Code	I4	5600
End of MSA Code Indicator	I4	Must be 0000

* At present, choices are limited to COASTAL or INTERIOR meteorology.
Note: All entries must begin in Column 1.

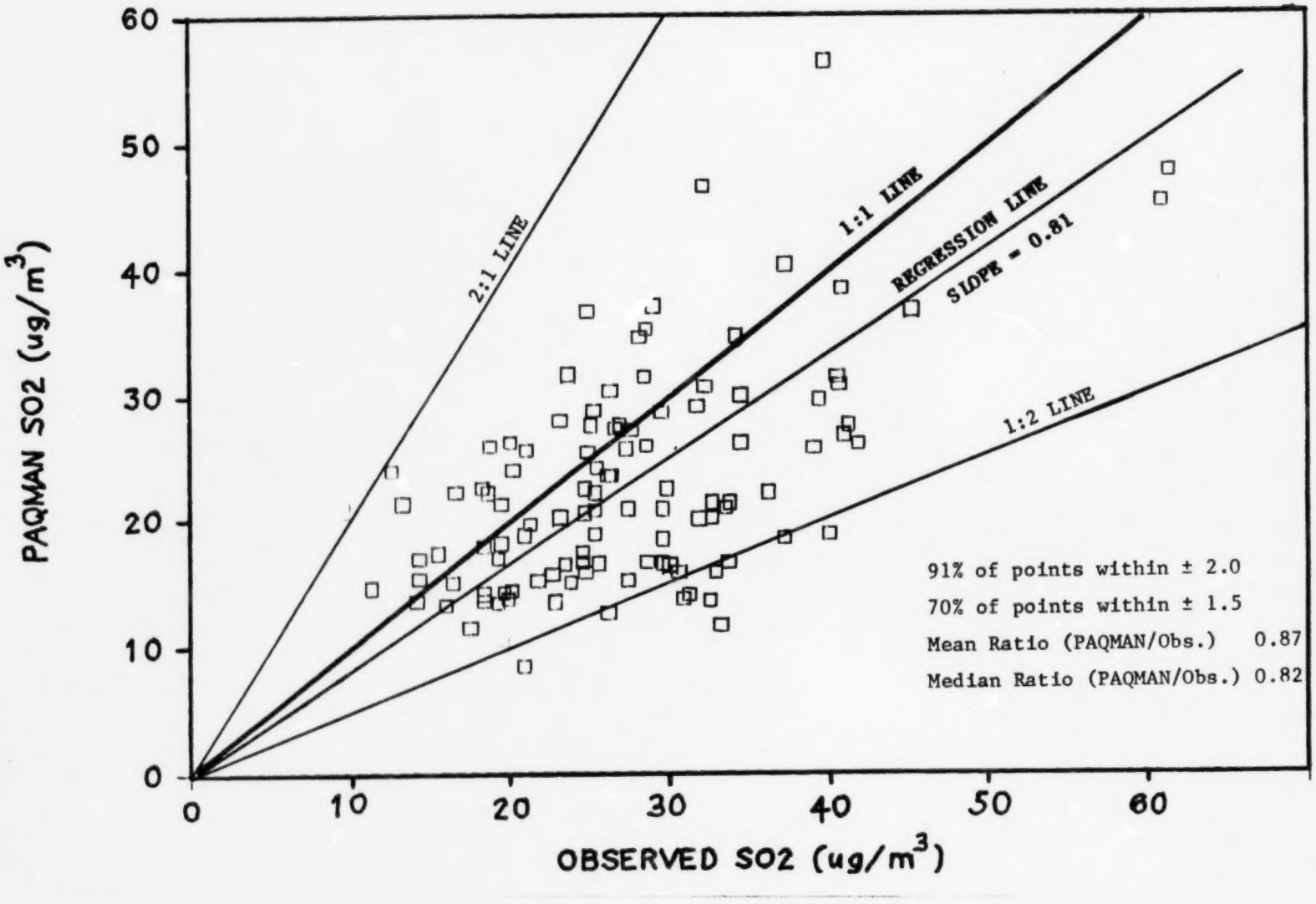


Figure 6. Comparison of Average PAQMAN and Average Observed SO_2 Concentration for 112 MSA'S.

3.0 PAQMAN SENSITIVITY ANALYSIS

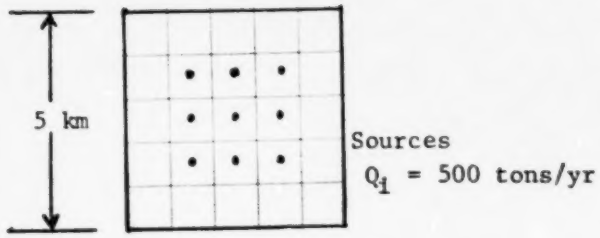
Test case comparisons performed between PAQMAN and CDM for the New Haven, CT and Pittsburgh, PA MSA's using 5 km^2 calculation grids indicated that PAQMAN values correlated well with CDM calculations, particularly for higher SO_2 levels (which were primarily due to area sources). Correlation coefficients were 0.90 and 0.80, respectively. Comparisons between PAQMAN values and monitored data (grid square averages) for Pittsburgh showed agreement generally within a factor of 2 as did MSA-averaged PAQMAN calculations and averaged observed values for all 112 MSA's (slope of 0.81 for regression forced through origin as shown in Figure 6).

These test cases, however, revealed some problems in the model that required further examination. The model predicted some very high SO_2 values at a few isolated "hot spots", particularly near large clusters of sources. In addition, comparisons with CDM for an individual MSA showed bias at the lower SO_2 levels (primarily due to point sources) which are linked to the direction - averaging technique (as opposed to specific wind-direction effects) applied in the development of the point source algorithms. Based upon these results, the following areas of uncertainty are noted and sensitivity analyses with regard to each item are described.

3.1 Sensitivity of PAQMAN Predictions to Grid Cell Size

As designed for the "85 Assessment, PAQMAN produces grid cells of 5x5 km encompassing a given MSA. Point source contributions to each grid centroid are computed; area sources within each grid square are aggregated and the contribution (grid square average) based on emission density in assigned to the grid centroid. Thus, the area source calculations are very dependent upon the grid cell size, as seen from Figure 5. As the size of the cell decreases, the area over which the emissions are aggregated decreases. At the same time, the number of sources which fall into a given grid cell is subject to change, depending on the location of the sources. The effect upon the area source calculation relative to a change in grid size will depend not only on the location of the sources, but even more importantly, on the distribution of emissions among these sources.

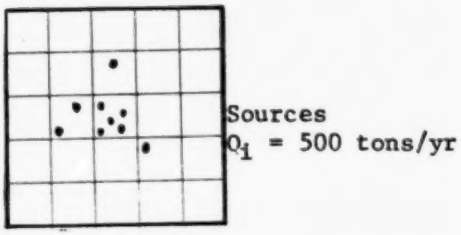
As a hypothetical example, let us suppose that a group of sources all with stack heights less than 200 ft. are distributed over a 5-km grid cell as shown in Figure 7a. Assume that each source emits 500 tons SO_2/yr. PAQMAN would predict an area source contribution over the grid of 47 $\mu g/m^3$. With 1-km grid spacing, the model would produce the distribution shown in Figure 7b, with a maximum concentration of 87 $\mu g/m^3$ at the center square of the 5x5 receptor grid, and an average of 19.3 $\mu g/m^3$ over the 5x5 grid. Redistributing the locations of the same sources as shown in Figure 7c would give the same concentration (47 $\mu g/m^3$) using a grid length of 5 km, and produce the distribution shown in Figure 7d for 1-km grid cells. The concentration of more sources falling within the central square of the 5x5 matrix results in the higher maximum of 167 $\mu g/m^3$, but concentrations at the outer edge of the 5x5 matrix are reduced and the overall average is about the same (19.5 $\mu g/m^3$). If we assume the same source orientation as in Figure 7c but redistribute the emission source strengths as shown in Figure 7e, the concentration distribution shifts as shown in Figure 7f, but again the overall average remains the same.



a.

4	8	13	8	4
8	33	33	33	8
13	33	87	33	13
8	33	33	33	8
4	8	13	8	4

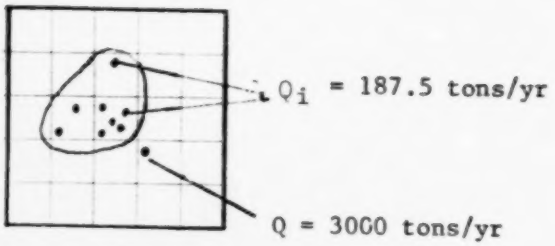
b.



c.

0	4	4	4	0
7	30	33	22	0
7	67	67	26	4
7	26	30	33	4
0	0	4	4	4

d.



e.

0	2	2	2	0
3	11	13	8	0
3	25	63	31	22
3	10	31	200	22
0	0	22	22	22

f.

Figure 7. Effect of source location and emission distribution as PAQMAN area source calculations using 1-km emission grids.

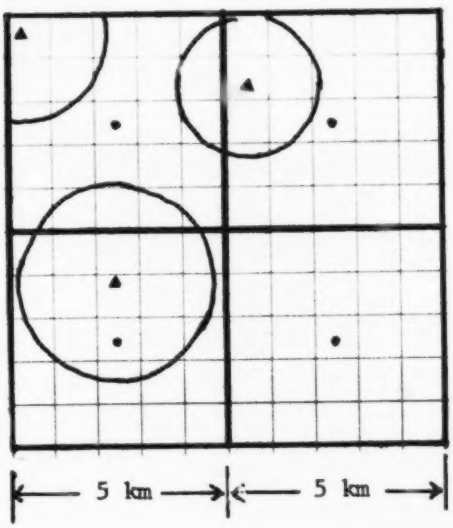
The difference between the predicted value of 47 $\mu g/m^3$ with 5-km spacing and the lower 5-km grid square averages (20 $\mu g/m^3$) obtained by averaging the 1-km estimates indicates that the area source algorithm may be underestimating the effect of neighboring grid cells. The model compares the emission density of a central grid cell (CED) with the average emission density (AED) of the surrounding 8 cells; if the relative difference (CED-AED) is greater than 10%, it is assumed that the adjacent grids have no effect on the central grid. The above results indicate that this tolerance may have to be adjusted (higher %). It is also possible that the area source algorithm relating the normalized concentration to the emission cell size (Figure 5) drops off too rapidly at the lower scale lengths, and this should be further investigated.

Point source contributions predicted by PAQMAN for each grid centroid are also sensitive to the grid size chosen. Smaller size grid cells (ie. 1 km vs. 5 km spacing) increase the number of receptors, and since the point source calculation is dependent upon the individual source-receptor distances (relative to the distance r_{max} of the maximum predicted concentration), the probability that some receptor will lie close to or at the location of an r_{max} (for any source) becomes larger. This is shown schematically in Figure 8a and 8b for 5-km and 1-km grid cells, respectively. Thus, the impacts of an individual point source may very well be underestimated with 5-km grids. This suggests that perhaps a similar concept of averaging the effect of a point source over the entire 5-km grid should be developed.

The optimal grid size with which to model, particularly for the area sources, is an interesting problem. Smaller grid spacing allows for more detail, but such detail may not be so important if the effects are aggregated over a large area such as an MSA. Since the interest in terms of materials damage assessment is in the aggregate, the effect of applying different grid size options in PAQMAN was analyzed in terms of SO_2 concentration for some of the larger cities. The results are shown in Table 4 for MSA-averaged values, which include the joint impact of area and point sources.

The MSA averages decrease with decreasing grid cell size (relative to 5 km), but show little change for larger cell sizes. This is likely due to the increase in the number of individual grids with predicted SO_2 values at the lower levels when the grid cell size is decreased, and again may indicate that the area source algorithm may be underestimating at the lower grid-scale levels. This is shown in Table 5 which presents the frequency distributions of the SO_2 concentrations predicted by PAQMAN for Pittsburgh, PA using 5-km and 1-km grid spacing. The distributions are very similar, heavily skewed toward lower SO_2 values with over 95% of the values in each case below 25 $\mu g/m^3$. This represents a far greater number of receptors (nearly 25 times) for the 1-km case (versus 5-km case), thus a lower overall average results with the 1-km grid spacing. Note, however, that the median values (50 %ile) are about the same.

The effect on the maximum concentration (not shown) is more pronounced than for the overall MSA average. This is because the maximum values are generally isolated "hot spots", having minimal effect on the overall MSA average particularly for the smaller grid scales.



Legend

▲ Point Sources

• Grid Centroids

— Distance to Maximum Concentration (r_{max})

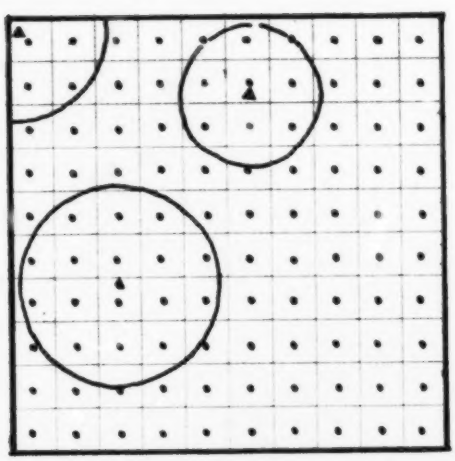


Figure 8. Schematic view showing effect of point source impact using 5-km vs. 1-km receptor grids.

Table 4. Effect of Grid Size On PAQMAN Predictions (MSA-Averaged Values)

	Ratio Relative to 5-km Value			
	1 km	2 km	10 km	20 km
Baltimore	0.53	0.66	0.95	1.03
Boston	0.83	0.90	1.09	0.93
Chicago	0.72	0.83	1.07	1.27
Cincinnati	0.87	0.93	1.01	0.98
Cleveland	0.86	0.92	1.07	0.99
New York	0.73	0.84	1.03	0.97
Philadelphia	0.68	0.80	1.10	1.08
Pittsburgh	0.89	0.94	1.01	0.97
Washington, DC	0.63	0.77	1.14	1.10
Average	0.75	0.84	1.05	1.04

Table 5. % Frequency Distributions of PAQMAN SO_2 Values for Pittsburgh, PA

	SO_2 Value ($\mu g/m^3$)	
Percentile	5-km Grid Spacing	1-km Grid Spacing
100	132.07	452.94
95	21.79	13.74
90	14.43	12.38
85	12.92	11.76
80	12.02	11.33
70	10.94	10.49
60	10.04	9.86
50	9.43	9.31
40	8.86	8.79
30	8.35	8.24
20	7.56	7.59
10	6.61	6.75
N	525	11349

While the SO_2 estimate is an important factor, other variables in the various damage functions including land use, building counts, time-of-wetness, etc. are affected by the grid size chosen in the model. Therefore, the sensitivity of actual damage estimates (both in terms of physical loss and economics) to different grid sizes should be examined.

3.2 Sensitivity of PAQMAN Predictions to the Designation of Sources as Area vs. Point Sources

In order to eliminate extensive manual manipulation of individual MSA emission inventories, an automated procedure that could readily be applied for all MSA's was developed in PAQMAN to segregate the emissions into area and point sources. As previously discussed, the criterion used to define a source as an area or point source is based on stack height. Stacks greater than 200 ft. are treated as point sources, those less than or equal to 200 ft. as area sources. The emissions from all area sources within a given grid cell are then aggregated. Point sources are treated individually, except for sources located within 0.1 km of each other in which case the emissions are summed and an emission-weighted average stack height is assumed in the point source calculation algorithms.

The choice of 200 ft. as the source-type criterion is not purely arbitrary. Comparison of point and area source calculations for a source assuming a range of stack heights (for the point-source algorithms) revealed that a source with a stack height of 200 ft. would produce a maximum ground-level concentration in the point-source mode equivalent to the concentration that would be predicted if it were assumed an area source using 5-km emission grids. Area source contributions are higher than corresponding maximum point source contributions for sources with stacks above 200 ft. Similar analysis assuming different emission grid sizes for the area source calculations suggests that the stack height criterion should be adjusted relative to the grid size chosen in the model, as shown in Table 6.

While the concept of defining a source as an area or point source based on stack height does have some merit, as shown above, the impact of a given source predicted at a receptor will be very sensitive to its treatment as an area or point source.* The effect of an area source in the model is averaged and assumed uniform over the 5-km grid square. The effect of a point source, however, is distance-dependent, with the maximum impact occuring at some distance (r_{max}) downwind from the source. Thus, for a 200-ft. stack, the point source contribution at a receptor (grid centroid) will be equivalent to the predicted area-source impact only if the source-receptor distance is equivalent to r_{max}. At distances less than or greater than r_{max}, the point source contribution will be less. Table 7 shows that the differences can become quite pronounced for a source located at the edge of a grid cell, particularly for the larger grid sizes. This effect becomes quite variable when several sources scattered about the grid cell are involved. Again, these differences suggest that point source effects should be averaged over the grid square, similar in concept to the way area source effects are represented in the model.

*This is true for most standard EPA models as well, including CDM. It should also be noted that many of the algorithms employed for characterizing dispersion from area sources in these models make simplifying assumptions in order to reduce the time needed to make the computations.

Table 6. Point Source Stack Heights Producing Maximum Ground-Level Concentrations Equivalent to Area Source Calculated Concentrations

PAQMAN Grid Size	Stack Height	
	Coastal	Interior
1 km	44m (144 ft)	34m (112 ft)
2 km	50m (164 ft)	39m (128 ft)
5 km	68m (223 ft)	50m (164 ft)
10 km	87m (285 ft)	68m (223 ft)
20 km	120m (394 ft)	90m (195 ft)

Table 7. PAQMAN Predictions (at Grid Centroid) for Point Source Located at Edge of Grid Cell Expressed as Ratio of χ/χ_{max}

	Coastal		Interior		
PAQMAN Grid Size (km)	Stack Height (m)	Ratio* (χ/χ_{max})	Stack Height (m)	Ratio* (χ/χ_{max})	Distance from Grid Centroid (km)
1	44	0.29	34	0.56	0.71
2	50	0.14	39	0.36	1.41
5	68	0.07	50	0.21	3.54
10	87	0.05	68	0.15	7.07
20	120	0.03	90	0.12	14.14

* Ratios illustrate that for a source located at the edge of a grid cell, PAQMAN will predict a significantly lower SO_2 value at the grid centroid if the source is treated as a point source verses an area source. The differences will be less pronounced for sources located closer to the grid center, and will be negligible at a distance r_{max} (defined as the distance from the source to the maximum ground-level concentration) away from the grid center.

The sensitivity of the point-area source definition was likely responsible for some of the isolated "hot spots" predicted by PAQMAN for some of the MSA's involved in the Assessment. Many of these cases involved a group or cluster of sources (industrial complexes in industrial type cities such as Cleveland, Baltimore, Gary-Hammond, Philadelphia) all with stack heights less than 200 ft., which all fell within the same grid square. The aggregation of emissions among these sources produced some rather high area-source contributions. Downwash is a frequent feature of such complexes with short-moderate stack heights, which can lead to very high concentrations. It is extremely difficult to verify such values since the concentrations generally occur close to the cluster of stacks on plant property (not considered "ambient air" in a regulatory sense) and monitoring data are not required and often non-existent. However, even if these high concentrations were verified, they are likely to be isolated effects, occurring close to the plant location. The automated aggregation procedure in PAQMAN, however, averages this effect over the entire grid square.

It is apparent that these clusters of sources should be treated differently. One solution could be to simply treat them as individual point sources; however, the dispersion characteristic of these sources are often quite different from isolated and/or more elevated sources. This option would also increase computer time since each of these sources would be handled separately in the model. Another approach could be to lower the stack height criterion, but the effect will depend on the range of stack heights and distribution of emissions among the sources involved in each case. This may, for example, eliminate a high predicted concentration for one city but have no effect on another. Adding an emissions criterion (in addition to stack height) would eliminate shorter stacks with very high emissions (say a 60 ft. stack emitting 2000 tons SO_2/year, for example) from being treated as area sources, but the dispersive properties of a release have no relationship to the release rate. The most feasible solution, from a scientific point of view, may be to model these sources separately, using a different model. However, this would involve site-specific analysis and data manipulation which, in terms of assessment, PAQMAN was specifically designed to prevent. Furthermore, in keeping within the context of assessment needs, the interest is in the aggregated effects over several MSA's. As previously mentioned, these "isolated" high concentrations do not have a significant impact on the overall MSA averages (unless, of course, critical materials happen to be located there).

3.3 Wind Direction Effects

One of the major assumptions inherent in the PAQMAN model is that local meteorology over a long-term, annual basis can be generalized into a regional representation. Three wind roses (New York, Pittsburgh and Cincinnati) were used in the parametric CDM runs. Results were directionally-averaged and combined into two separate categories, coastal (New York) and interior (blend of Pittsburgh and Cincinnati), resulting in separate sets of dispersion algorithms for coastal and interior locations.

It was thought that this methodology would not introduce any net bias for a large number of sources scattered around an urban area. However, test case studies comparing PAQMAN calculations with CDM results for individual MSA's reflected some bias, particularly at the lower SO_2 levels (point sources and for cities where major point sources were concentrated in one given area. This effect is presented in Figures 9 and 10 for New Haven, CT and Pittsburgh, PA respectively, which show a comparison between PAQMAN and CDM point source calculations.

For New Haven (Figure 9), PAQMAN overestimated relative to CDM at the very lowest SO_2 levels and underpredicted for the higher point-source levels (which were still quite low in comparison to area source impacts). The correlation was 0.58 for the point source contributions. (Correlation between area source contributions was 0.94) The underprediction is explained by the fact that New Haven is affected by major point sources to the southwest, as shown in Figure 11. With prevailing winds out of the southwest, the effect of these major sources is underestimated by the directional-averaging technique that was applied in developing the PAQMAN point source algorithms.

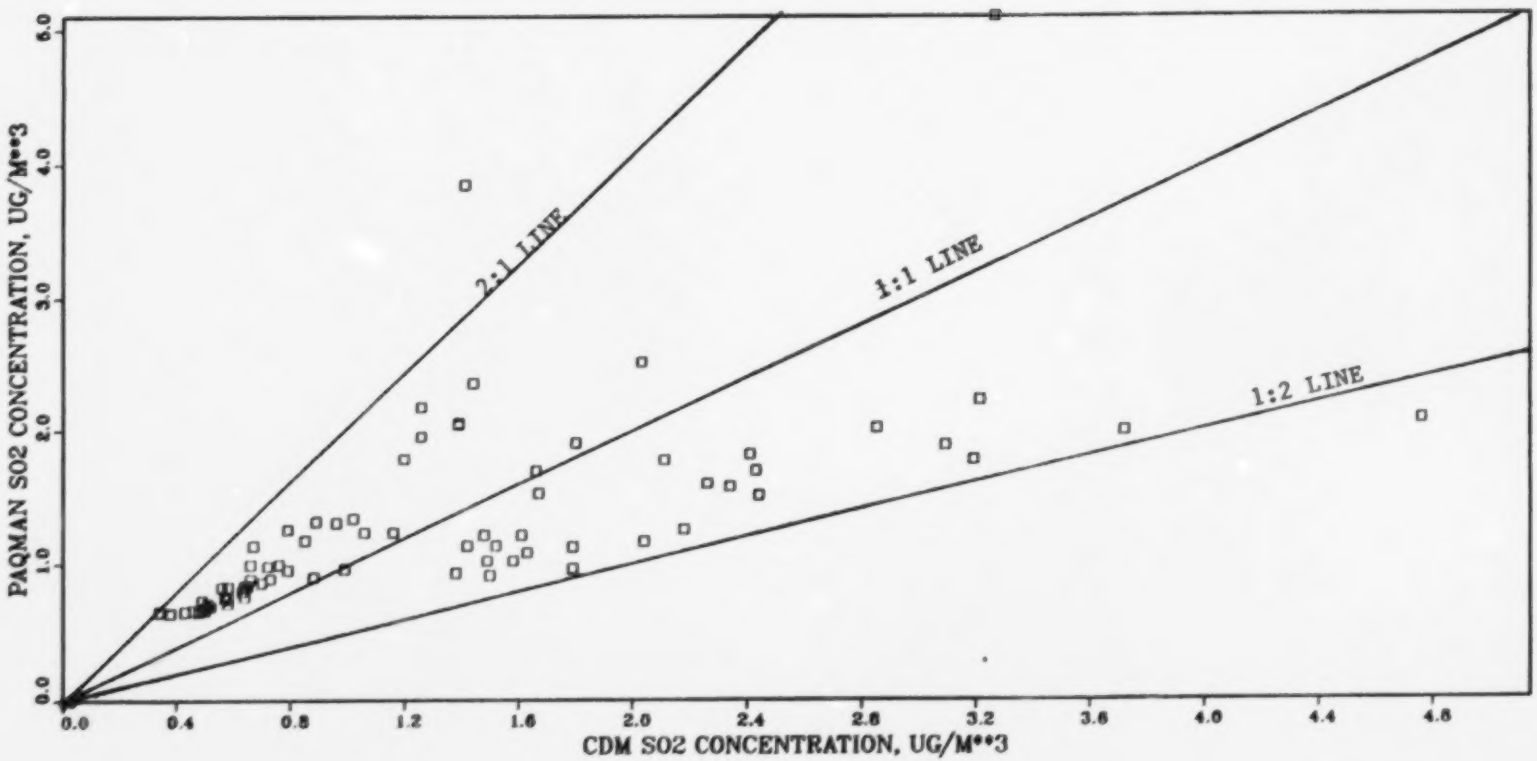


Figure 9. Comparison of PAQMAN vs. CDM SO_2 Concentration Estimates for New Haven, CT - Point Sources Only

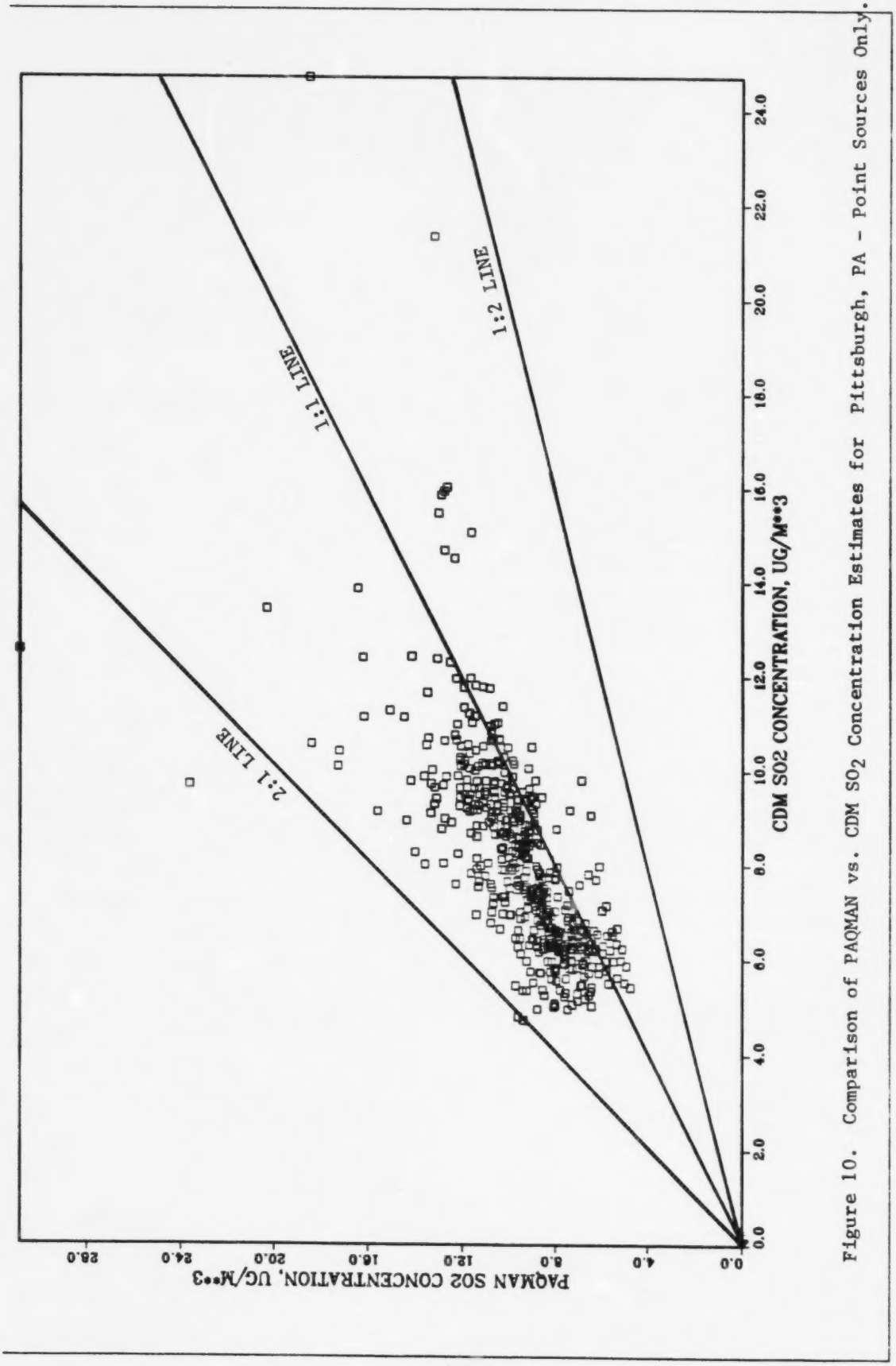


Figure 10. Comparison of PAQMAN vs. CDM SO_2 Concentration Estimates for Pittsburgh, PA - Point Sources Only.

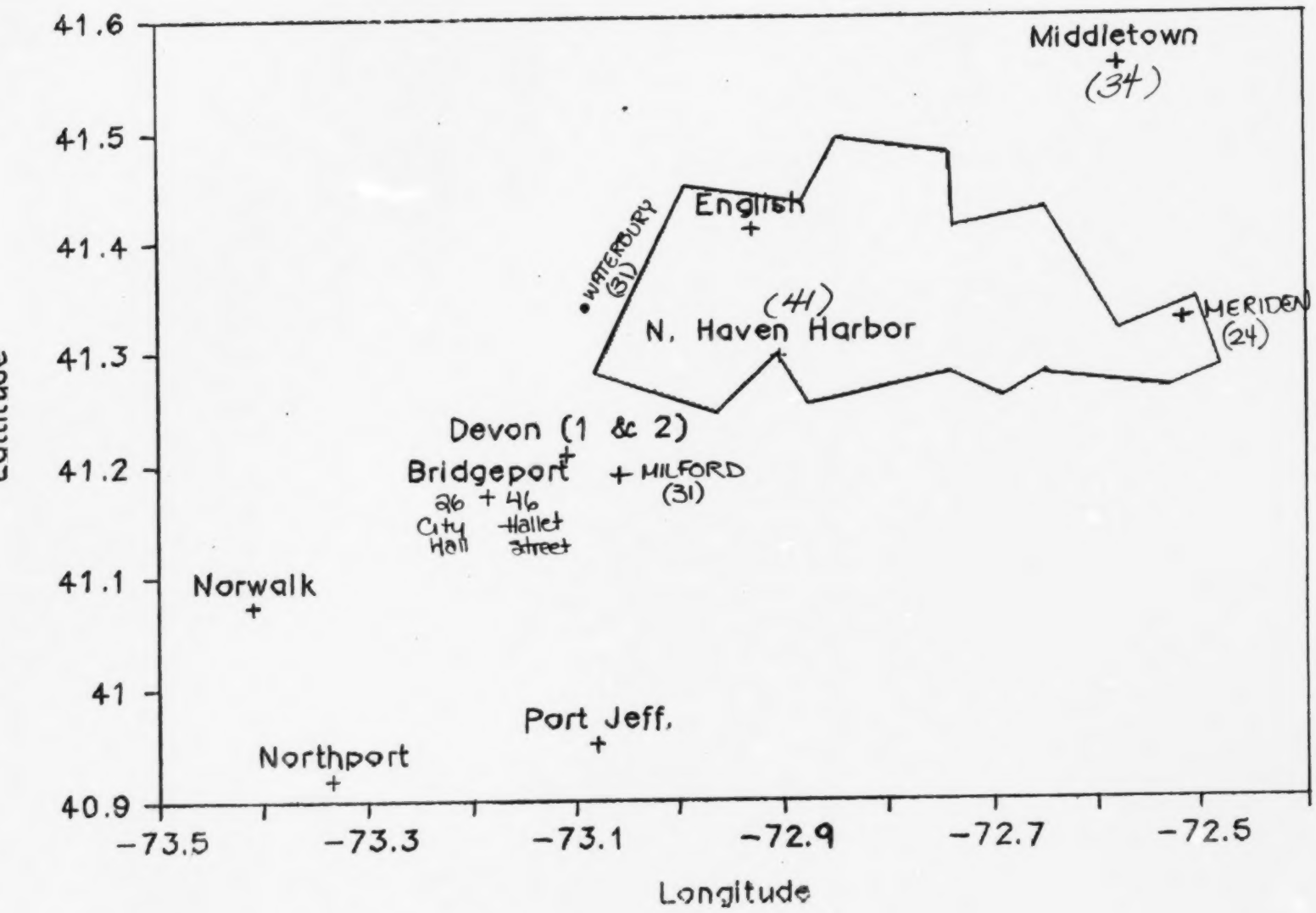


Figure 11. Schematic of the major point sources surrounding New Haven, CT

In contrast, Pittsburgh has major point sources primarily to the east and southeast of the city. Therefore, PAQMAN tends to overpredict their contribution relative to CDM (Figure 10) since prevailing winds are generally westerly. The correlation was 0.66 for the point source contributions (0.96 for area source contributions in Pittsburgh). The higher correlations for the area source comparisons between the two models indicates that site-specific wind direction affects are not as important for the area source dispersion algorithms.

The errors induced by the directional averaging in PAQMAN may very well balance out in the overall aggregated Assessment over all 112 MSA's. However, the tendency toward over- and underprediction of the point source estimates (relative to CDM) suggests that wind-directional effects are important and should be considered. This could be accomplished in the PAQMAN code, but would involve similar calculations that are presently applied in existing models such as CDM. Since the major attributes of PAQMAN are in its automated development of receptor grids encompassing the MSA, the segregation of source type and the rapid assessment of area sources*, there concepts could be incorporated directly within CDM, although it would involve some revisions to the CDM code. Regionally representative wind rose-stability frequency distributions could be utilized as input for the CDM point source calculations as opposed to site-specific meteorology, with an indicator flag set by the user to invoke the appropriate meterological data set. Since the development of the receptor grids, aggregation of sources and area source algorithms in PAQMAN all exist as subroutines, these calculations can be incorporated similarly within the CDM code. Some of these modifications were successfully made for the test-case comparison studies between CDM and PAQMAN.

3.4 Alternative Dispersion Coefficients

As discussed in Section 2.2, the algorithms applied to describe the dispersion from individual point sources in PAQMAN are driven by relationships between stack height, maximum ground-level SO_2 concentration and the distance downwind of the maximum concentration. These were derived from parametric runs using the CDM model with the McElroy-Pooler (M-P)[8] dispersion coefficients. Although these coefficients have been recommended by EPA for modeling point sources in an urban environment, it is important to examine whether the parameterization will be valid using another set of dispersion coefficients.

Due to their wide acceptance and use in dispersion modeling, the dispersion coefficients recommended by Briggs[9] were chosen. A comparison between the Briggs' and McElroy-Pooler vertical dispersion coeffiecients (σ_z) are presented in Figure 12. It is readily apparent that σ_z values for the McElroy-Pooler curves are larger, particularly for the more unstable cases. Thus, a plume would reach the ground at distances closer to tne source than would be predicted by the Briggs' coefficients.

In order to account for increased turbulence in urban areas, the Briggs' coefficeints were increased by one stability class upwards (decreasing stability), except for the most unstable case (Class A), in the parametric CDM

*The area source calculation algorithms in CDM require a significant amount of computer run time, particularly when a large number of area sources are involved.

runs. A similar procedure is applied in the standard form of the CDM model using the Pasquill-Gifford dispersion coefficients[4]. As in the initial parametric CDM runs, plume rise was calculated according to Briggs, an experimental decay (3-hour half life) was assumed and directional-averaging of results was applied.

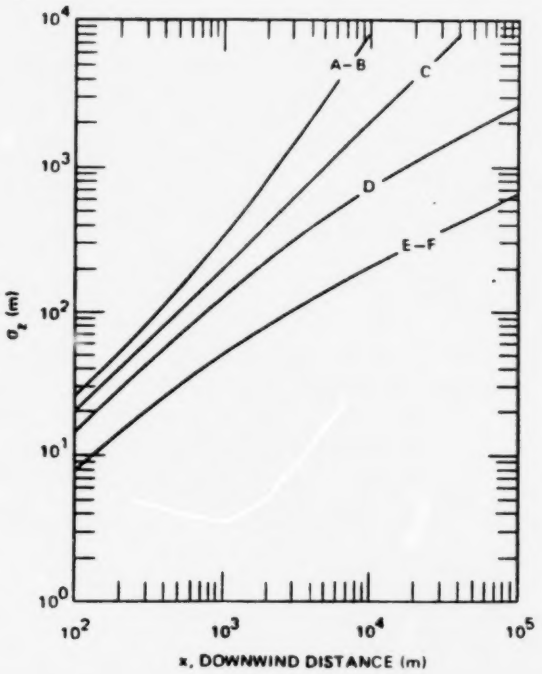
The results of the parametric runs with Briggs' coefficients revealed relationships similar to those established with the McElroy-Pooler dispersion algorithms. Maximum ground-level SO_2 concentration (/Q) was found to be an inverse-squared function of stack height (Figure 13) and the distance to the maximum concentration (r_{max}) a function of stack height (Figure 14). The downwind decrease of concentration relative to the maximum was related to the ratio of downwind distance (r) to the distance of the maximum concentration (r_{max}) as shown in Figure 15.

One of the underlying assumptions of the PAQMAN methodology is that all stack heights can be generalized into a single representation. This certainly was apparent with the McElroy-Pooler curves (see Figure 4). The results using the Briggs' algorithms, however, indicated differences in downwind dispersion characteristics with different stack heights. Figure 16 shows that a spread of a factor of 2 occurs at a ratio (χ/χ_{max}) of around 0.2. (A factor of 2 difference was found at a χ/χ_{max} of 0.01 for the McElroy-Pooler curves at which point absolute SO_2 levels are small and the error unimportant). Analyses with all three wind roses showed that the differences were systematic, with the downwind drop off in concentrations sharpest for the lower stack heights.

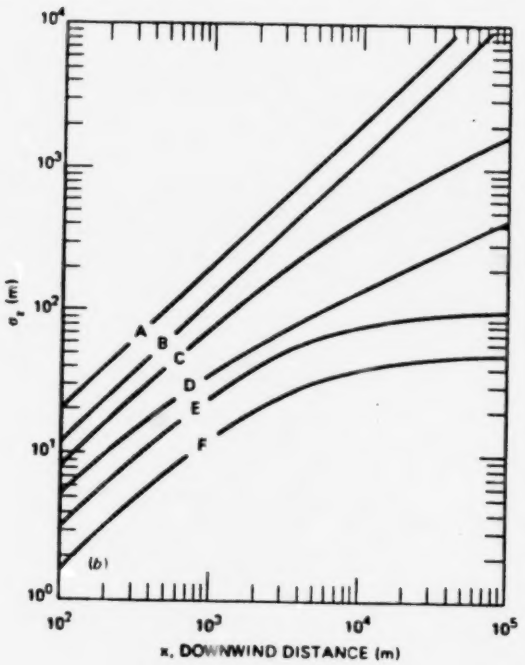
These results suggest that perhaps separate algorithms describing the decay of concentration downwind of the maximum be developed for shorter versus taller stacks. However, when the effects are analyzed across an entire MSA, the differences described above do not appear to be greatly significant. A comparison of PAQMAN runs for various MSA's applying both the McElroy-Pooler and Briggs' algorithms in the point source calculations revealed only minor differences for the most part for larger MSA's. Greater differences were found for smaller MSA's where individual point source effects are likely to have a more important effect on the overall MSA average, although absolute values are still quite small. Examples are shown in Table 8 for New Haven and Pittsburgh. Correlation coefficients between the M-P and Briggs values considering the total (area and point source) contribution are very high (0.97 and 0.98, respectively), but the MSA average with Brigg's was 30% higher than with the M-P coefficeints for New Haven, and 14% higher for Pittsburgh. Examining the point source contributions only clearly shows the more pronounced differences for the smaller MSA's such as New Haven where point source effects are more significant on the whole. The correlation coefficients are 0.77 for New Haven and 0.97 for Pittsburgh, with the MSA-average over 50% higher for the Brigg's sigmas than the M-P values for New Haven but only 16% higher for Pittsburgh.

3.5 Terrain Effects

The PAQMAN model (as well as CDM) does not account for terrain effects, and its applicability to urban areas in complex terrain (mountainous or hilly) is questionable and uncertain. There are several MSA's in the Northeastern



a. McElroy - Pooler (Urban)



b. Brigg's Rural

Figure 12. Comparison of McElroy - Pooler and Brigg's Rural Vertical Dispersion Coefficients (σ_z).

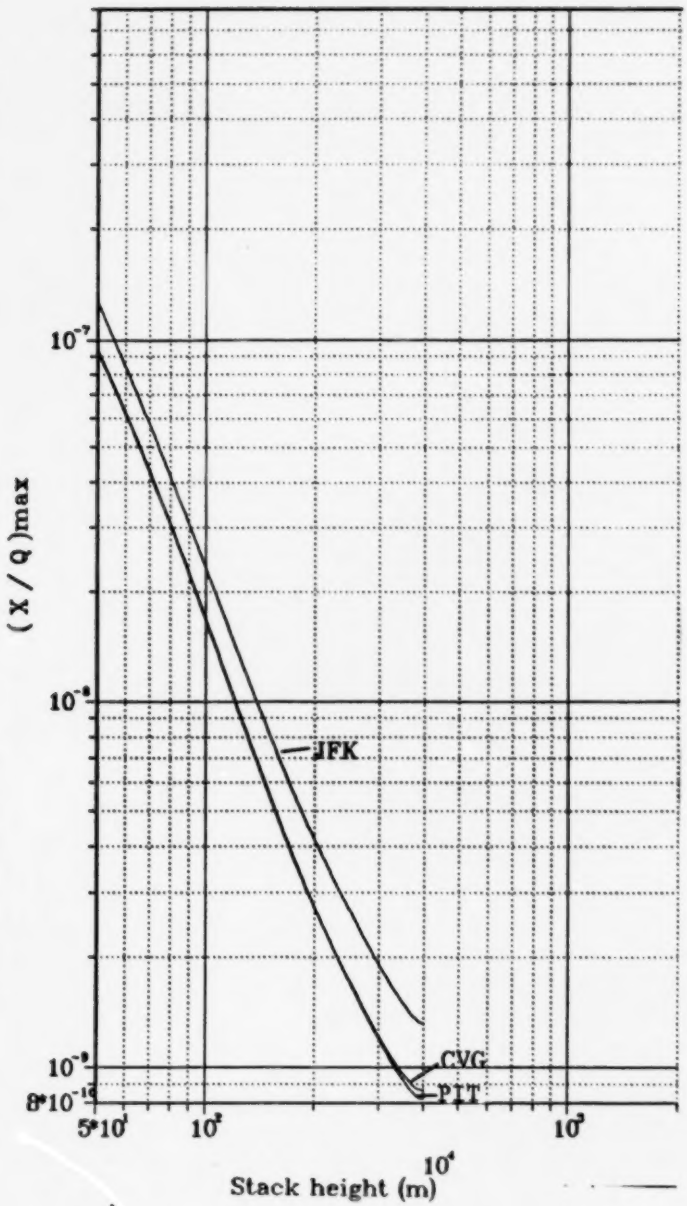


Figure 13. Max. Concentration vs. Stack Height
CDM Model
Briggs' Rural σ's (adjusted upward by one stability class)

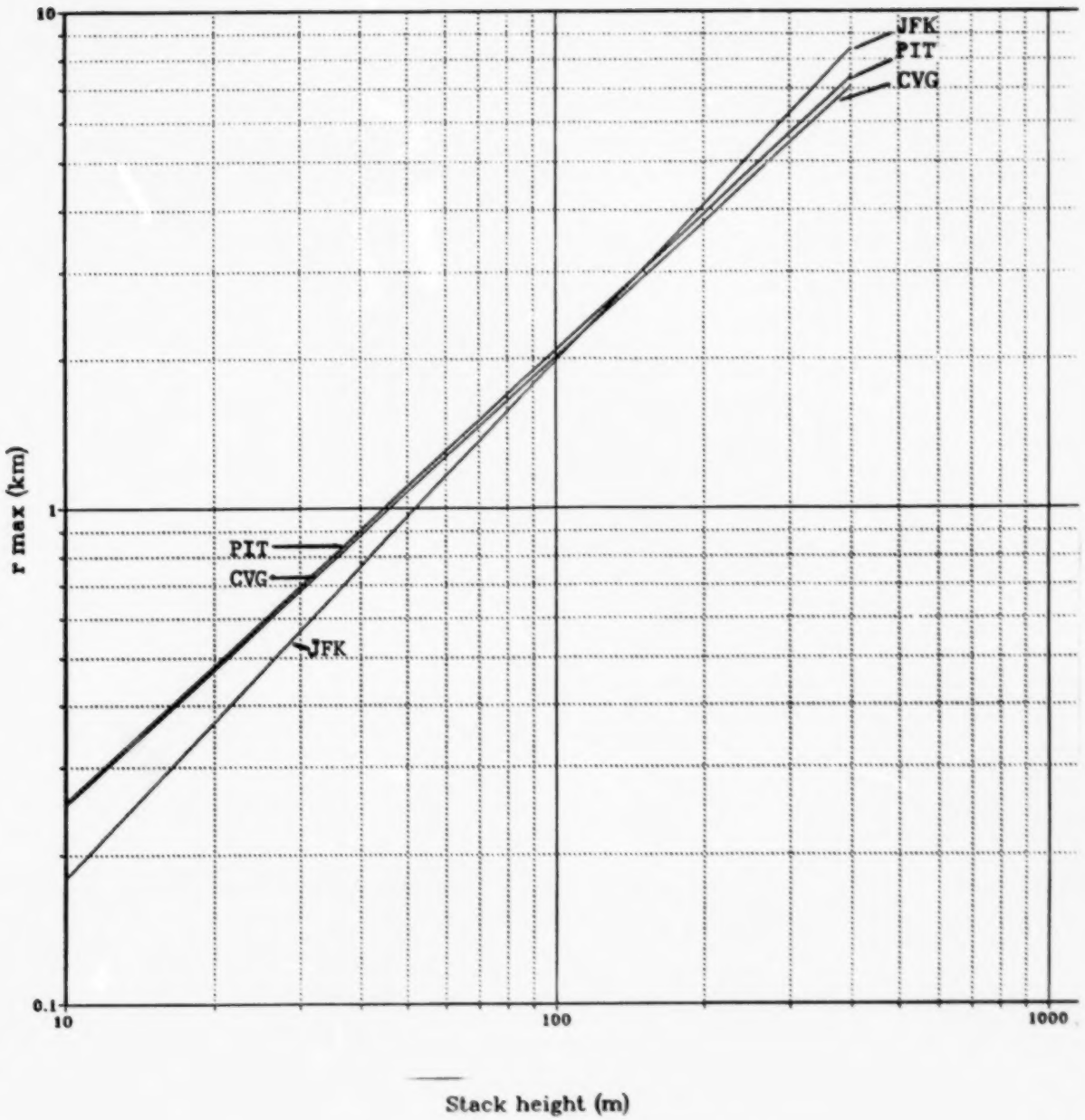


Figure 14. Downwind Distance to Maximum Concentration
CDM Model
Briggs' Rural σ's (adjusted upward by one stability class)

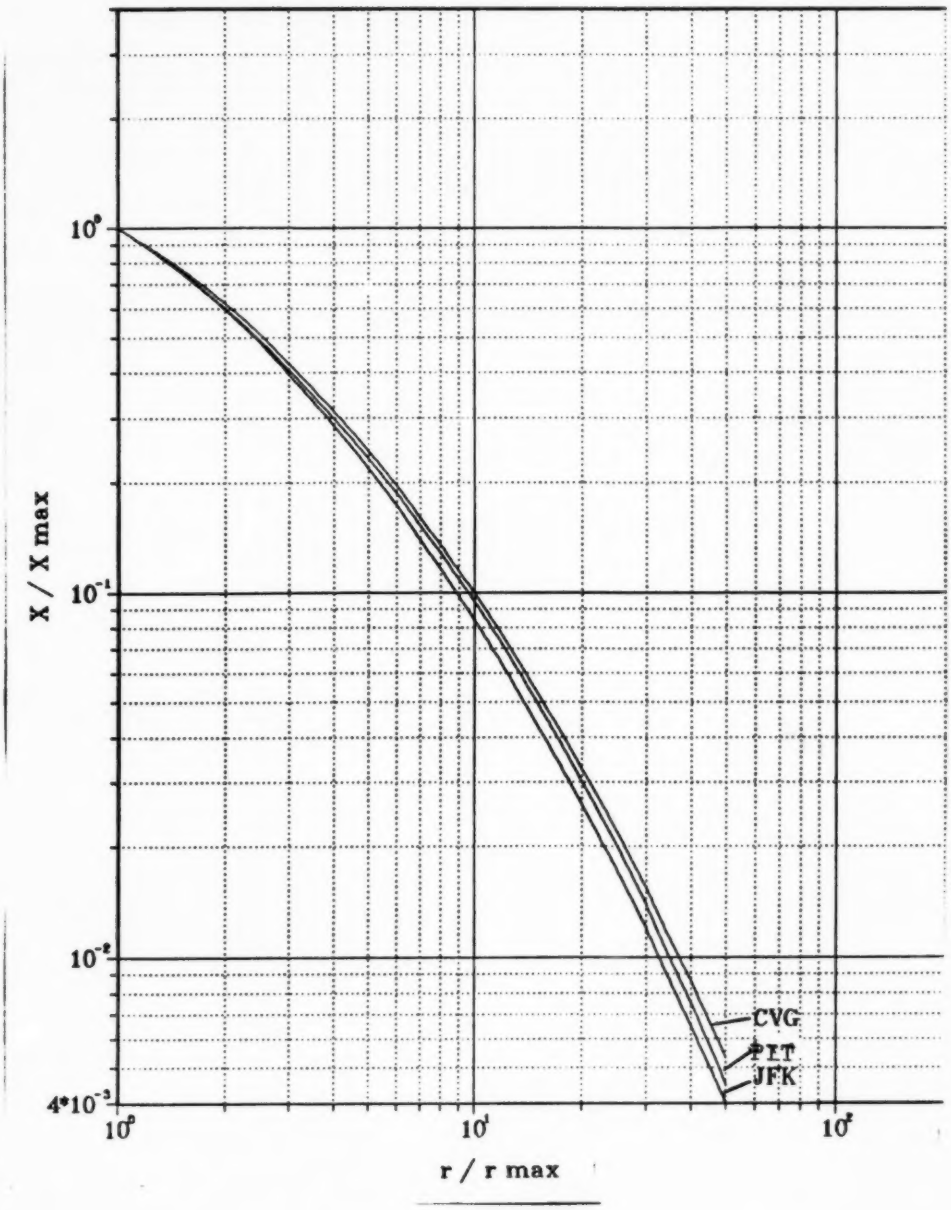


Figure 15. Concentration Ratio vs. Downwind Distance
CDM Model
Briggs' Rural σ's (adjusted upwards by one stability class)

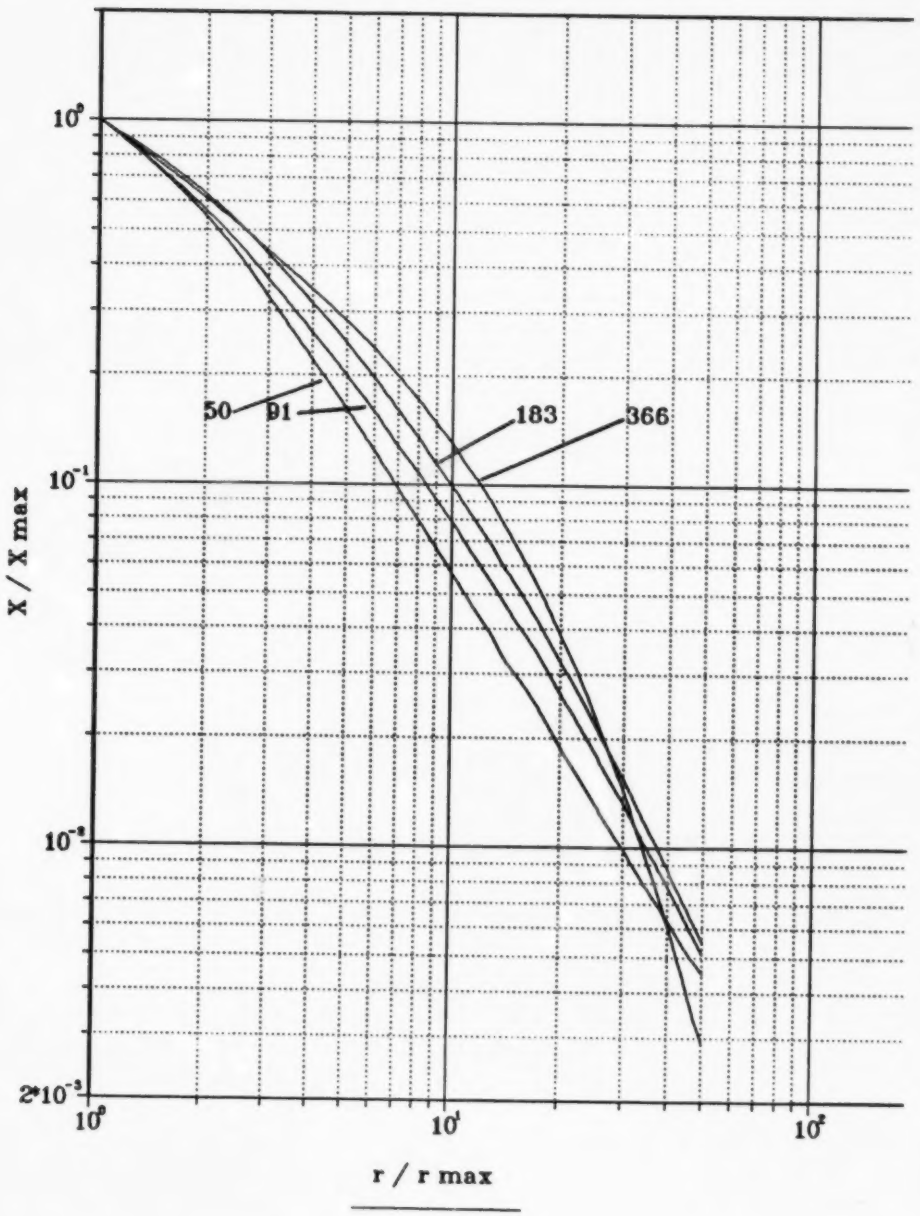


Figure 16. Concentration Ratio Vs. Distance Ratio
PIT Wind Rose - Varying H_s (m)
Briggs' Rural σ's (adjusted upward by one stability class)

Table 8 Comparison of PAQMAN SO_2 Calculations Based on McElroy-Pooler vs. Briggs Sigmas.

New Haven, CT

	Total* Contribution		Point-Source Contribution	
	M-P σ's	Briggs σ's	M-P σ's	Briggs σ's
MSA-Average	2.00	2.68	1.33	2.02
Maximum	14.68	14.41	5.10	4.06
Minimum	0.65	0.92	0.64	0.92
90th %ile	3.76	4.29	2.05	3.22
75th %ile	2.19	3.00	1.69	2.49
50th %ile	1.34	2.02	1.13	1.79
25th %ile	0.88	1.49	0.84	1.46
Correlation	0.97		0.77	

Pittsburgh, PA

	Total* Contribution		Point-Source Contribution	
	M-P σ's	Briggs σ's	M-P σ's	Briggs σ's
MSA-Average	10.98	12.48	9.44	10.94
Maximum	132.07	135.94	30.87	35.22
Minimum	4.58	3.94	4.58	3.94
90th %ile	14.43	17.87	12.13	15.25
75th %ile	11.45	13.58	10.76	12.94
50th %ile	9.43	10.61	9.26	10.37
25th %ile	7.96	8.62	7.85	8.44
Correlation	0.98		0.97	

* Total = Area Source + Point Source.

quadrant of the U.S., to which the model was applied in the "85 Assessment which can be classified as hilly, including Pittsburgh, PA and Huntington, WV to name a few. CDM is strictly a flat-terrain model; thus an alternative model should be mimiced and/or applied for locations where terrain effects are important.

3.6 Model - Observed Data Comparisons

The performance of an air quality model is generally evaluated by comparing predicted concentration values with observed data. Although monitoring data may not always be representative of reality, they are the only way to relate modeled values to some sort of "physical reality".

SO_2 monitoring data were acquired from the U.S. EPA's National Aerometric Data Bank for the Northeastern quadrant of the U.S., over the period 1976-1984. All measurement methods were considered except sulfation plate-type deposit gauges. These data were acquired as quarterly averages, then averaged over the entire time period in order to derive the maximum possible number of annual average estimates. (Many stations had relatively long periods of missing data, which often invalidated the annual average estimates in a given year; combining quarters from various years alleviates this problem as long as there are no strong long-term trends in the data.)

Annual average estimates were derived from over 100 cities in the Northeastern U.S. following the above protocol. Since many cities had a limited number of monitors (many had only one), comparisons between measured and PAQMAN-predicted SO_2 concentrations were performed only for the larger (major) cities where more monitoring data were available. In addition, since PAQMAN predicts for grid centroids only, comparisons for the same location (in space) were seldom possible, although PAQMAN area source contributions represent the average over a grid square. Therefore, comparisons were made between predicted values and observed values which fell within the same modeled grid square. In situations where several monitors fell within the same cell, grid-square averages were used.

Results of various cities are plotted in Figures 17-25, and summarized in Table 9. Model predictions are within a factor of ± 2 of observed values at all locations, with a few outliers, and within a factor of ± 1.5 over 70% of the time in seven of the nine cities analyzed. The mean ratio of predicted to observed values over the nine cities is 1.17, the median value is 1.03. Linear regressions (forced through the origin) with the PAQMAN value as the dependent variable indicated slopes ranging from 0.73 (New York City) to as high as 1.52 (Chicago), with an average slope of 1.11.

The gross outliers for Baltimore and Washington resulted from a power plant consisting of 5 "co-located" stacks of 161 ft., emitting a total of over 15,000 tons SO_2/year. Under the 200-ft. stack height criterion, PAQMAN treats these sources as an area source resulting in a very high predicted SO_2 concentration over the grid square. Assuming these sources to be point sources would have yielded a maximum input of 178 $\mu g/m^3$ at a distance of 0.21 km from the source (PAQMAN would aggregate the emissions to a single emission-weighted stack height of 161 ft. since the stacks are within 0.1 km of each other), but values of only 5 $\mu g/m^3$ and 15 $\mu g/m^3$ (21 and 31 $\mu g/m^3$ including background) at the grid

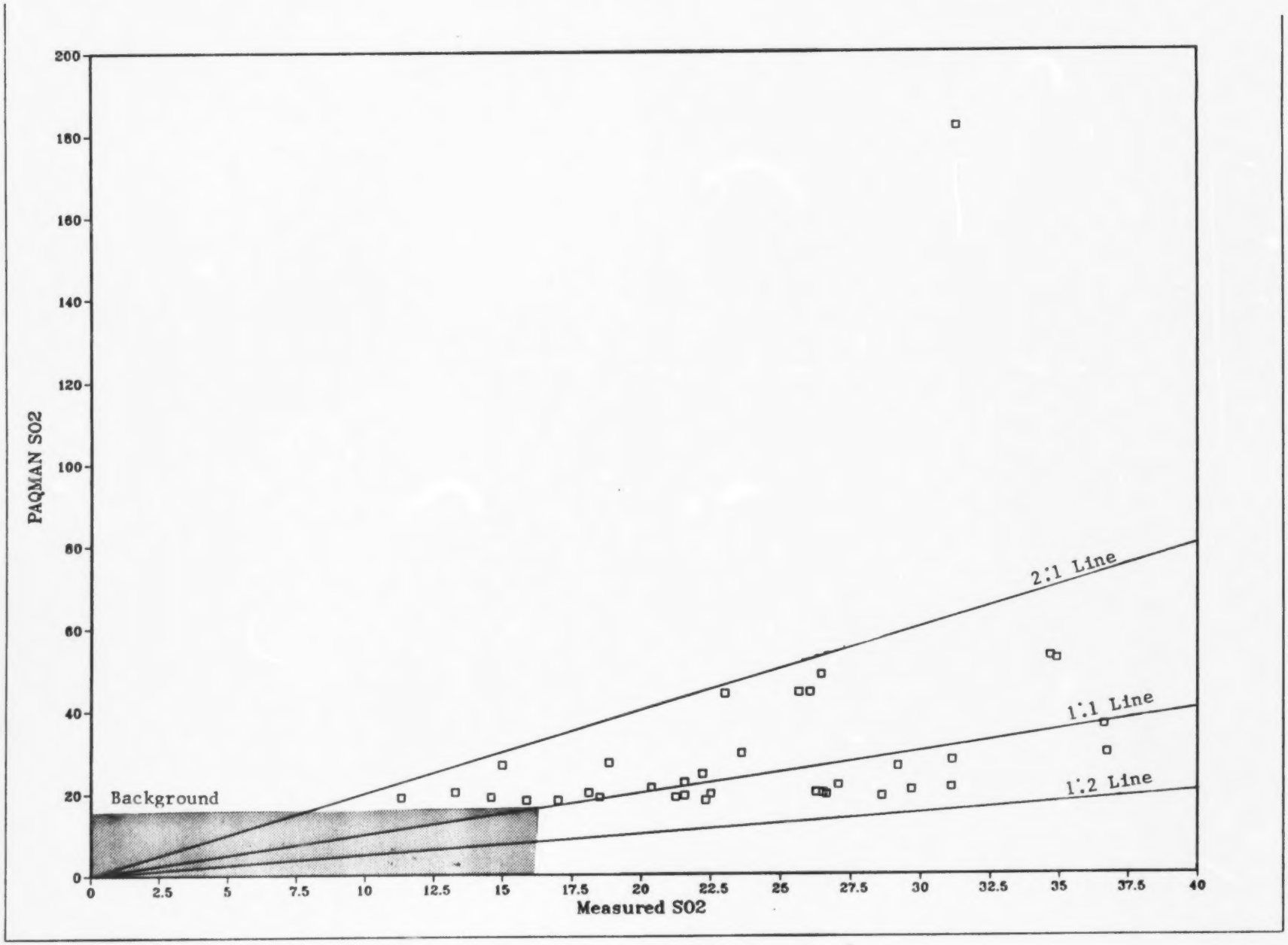


Figure 17. Comparison of PAOMAN vs. measured SO_2 - Baltimore, MD.

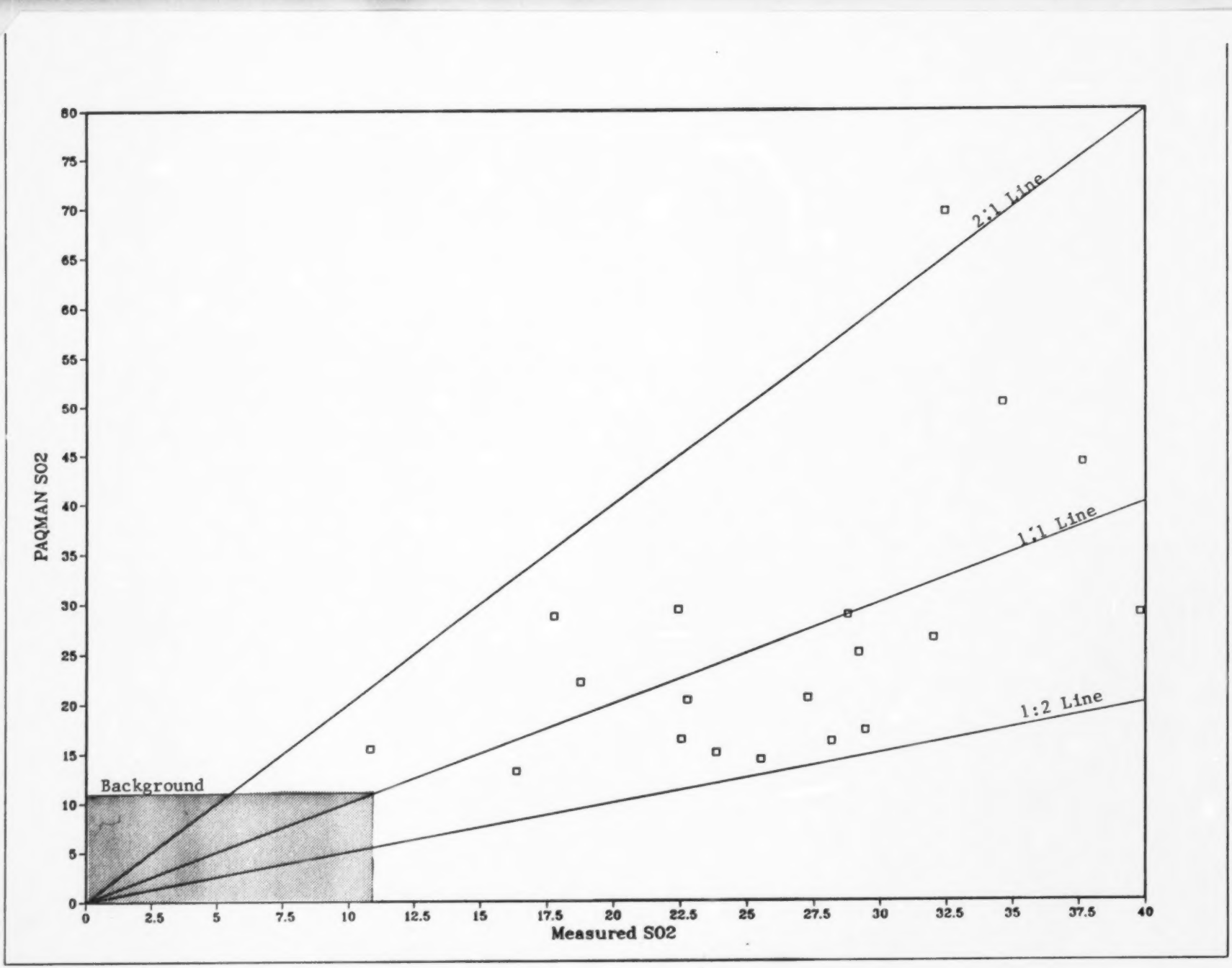


Figure 18. Comparison of PAQMAN vs. measured SO_2 - Boston, MA

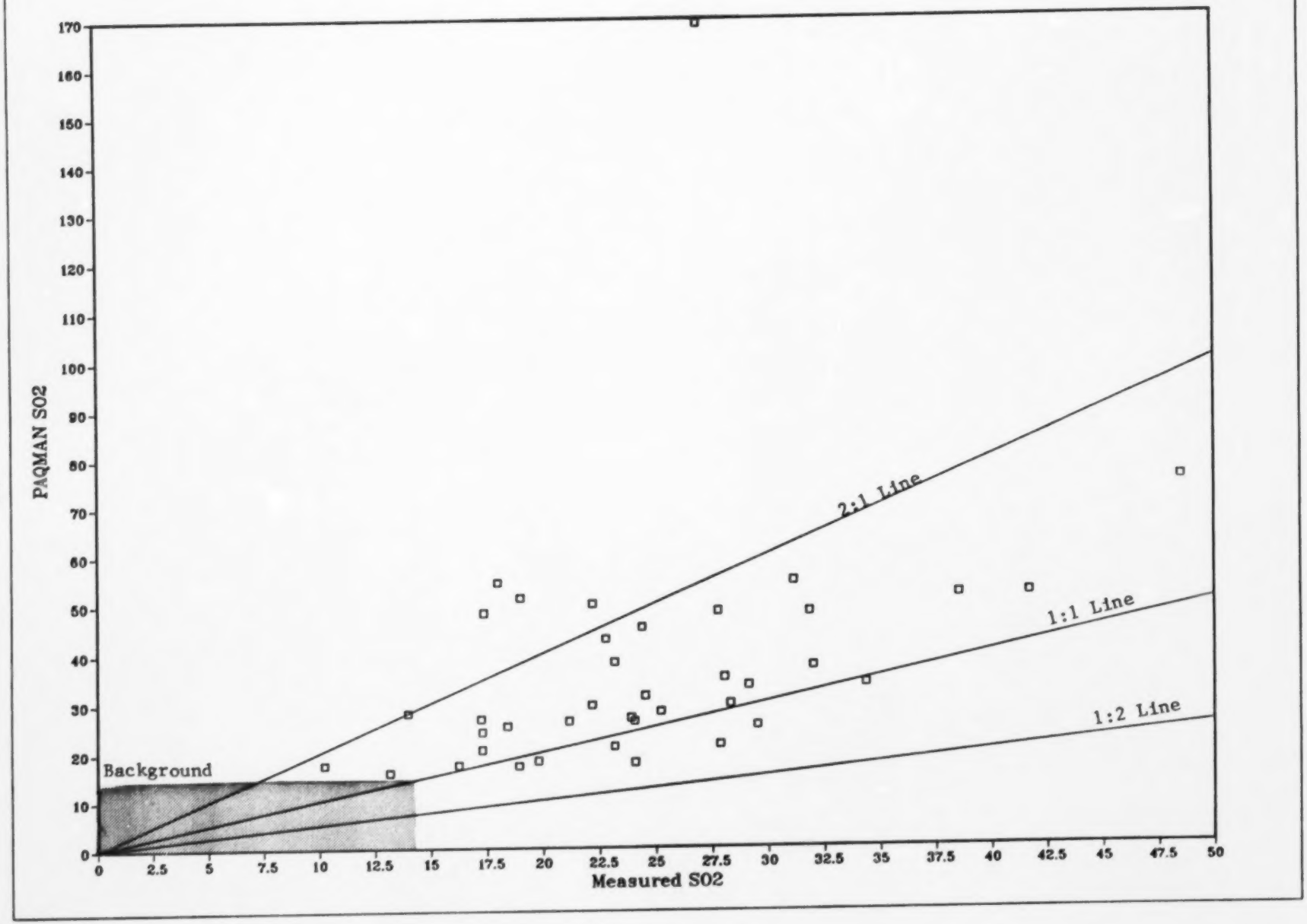


Figure 19. Comparison of PAQMAN vs. measured SO_2 - Chicago, Il

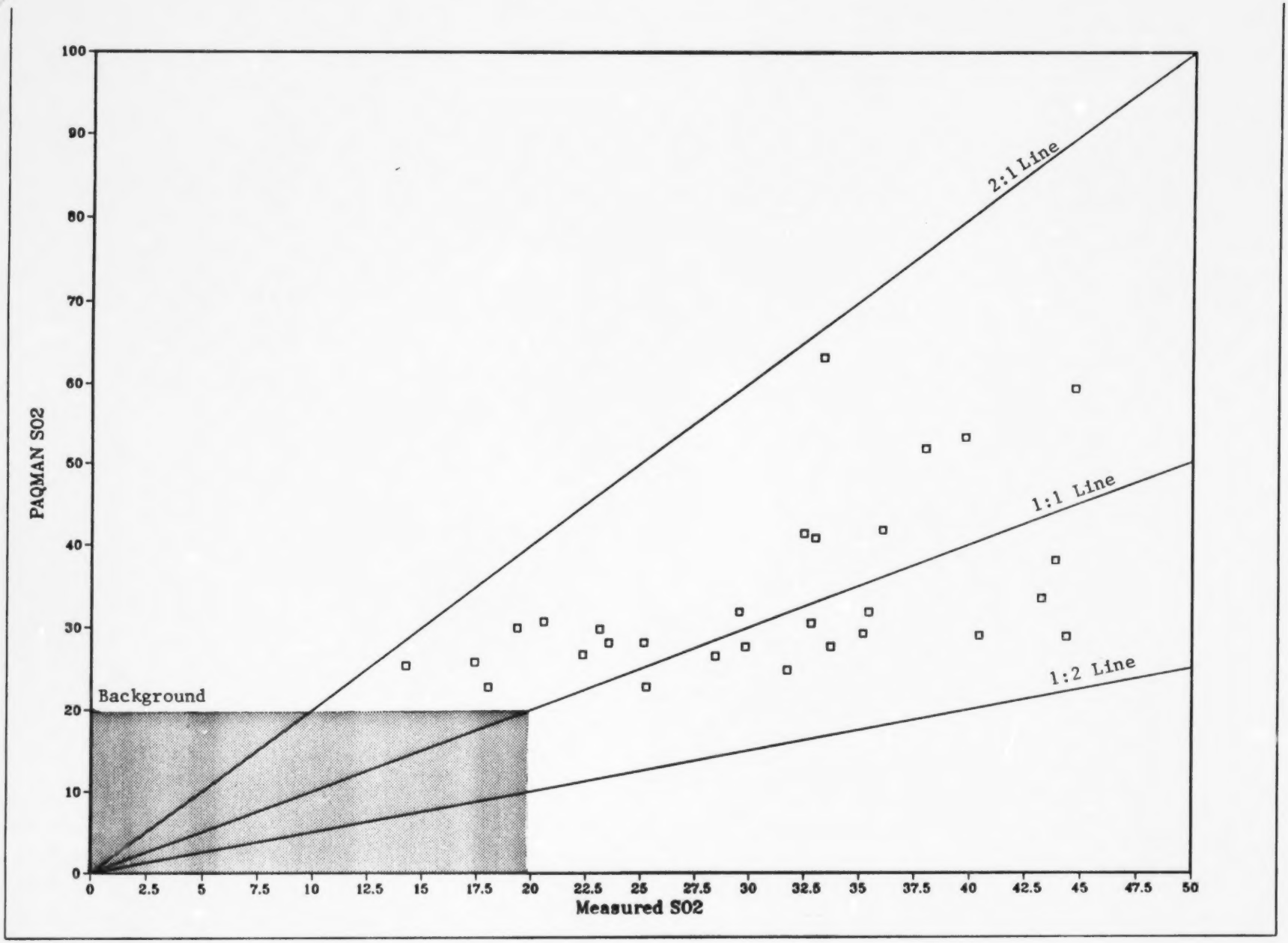


Figure 20. Comparison of PAQMAN vs. measured SO_2 - Cincinnati, OH

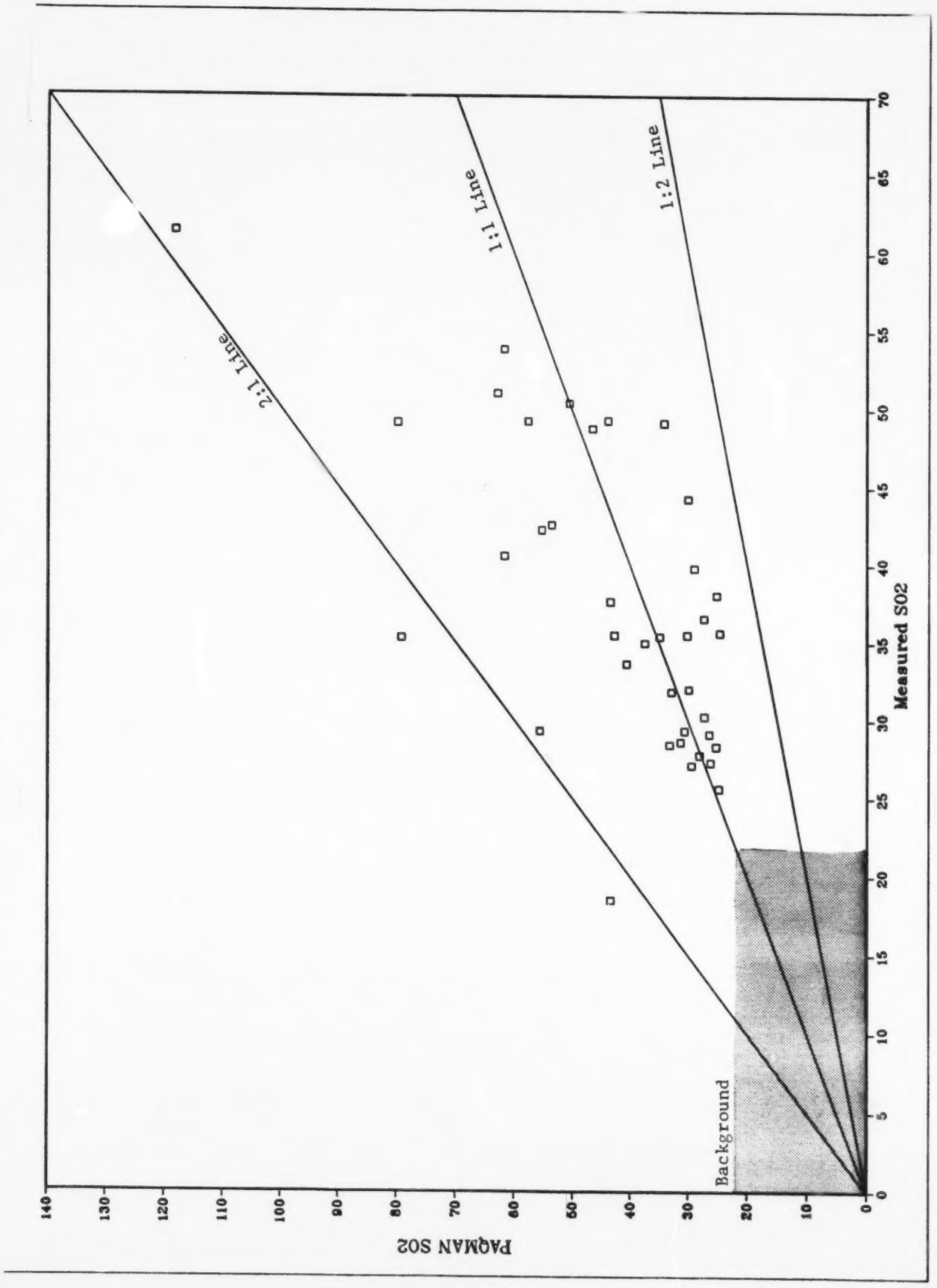


Figure 21. Comparison of PAQMAN vs. measured SO_2 - Cleveland, OH

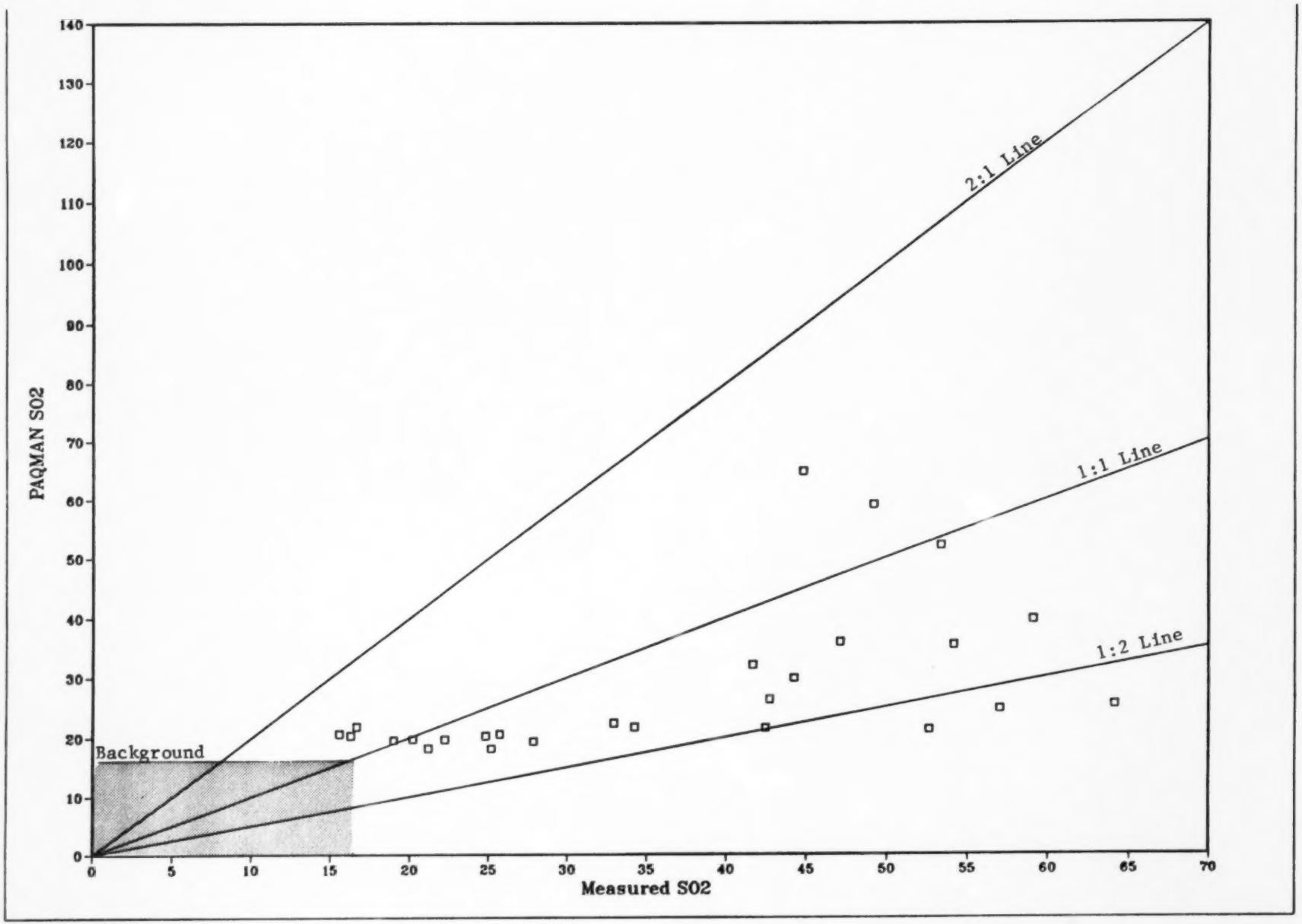


Figure 22. Comparison of PAQMAN vs. measured SO_2-New York City, NY

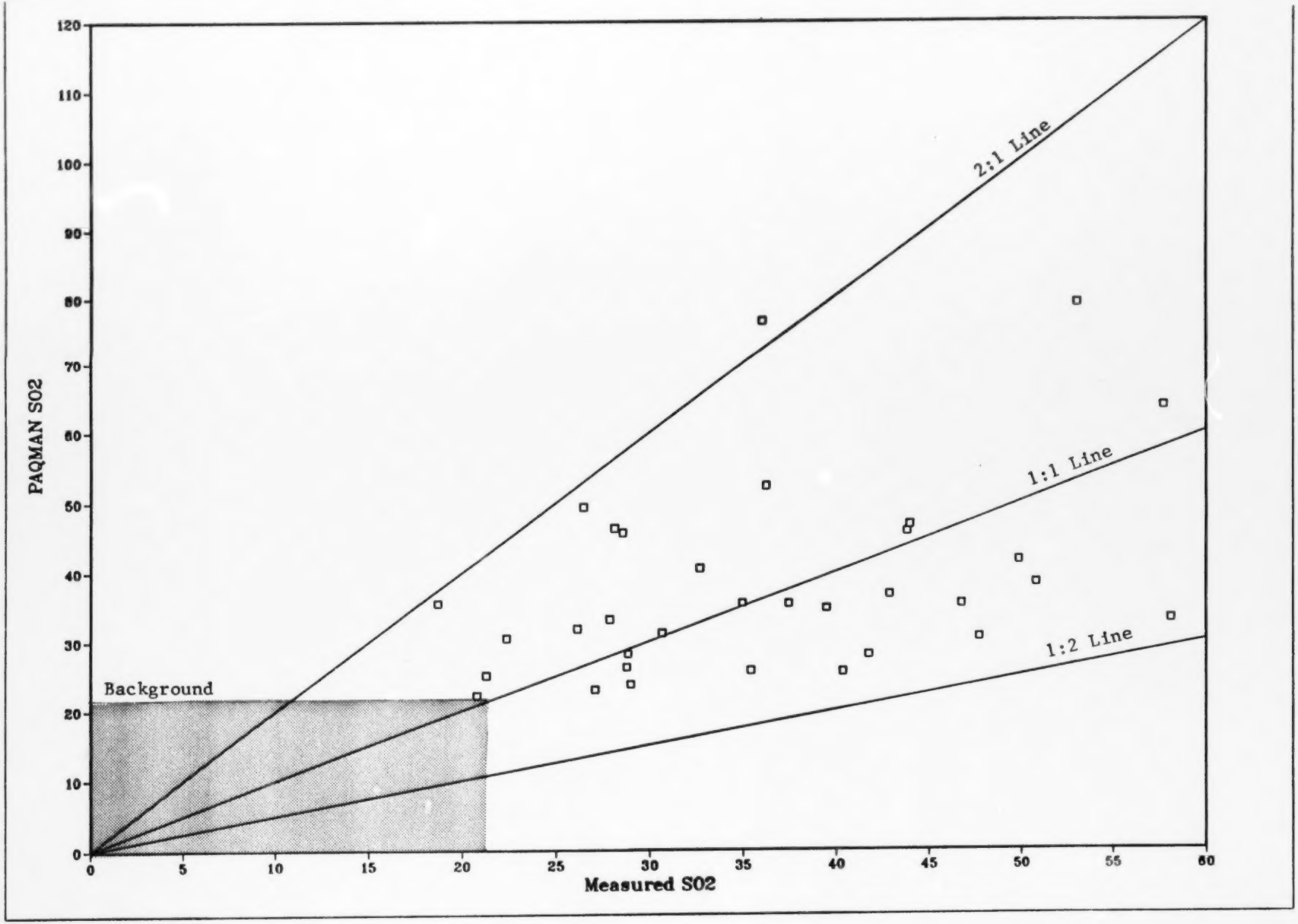


Figure 23. Comparison of PAQMAN vs. measured SO_2 - Philadelphia, PA

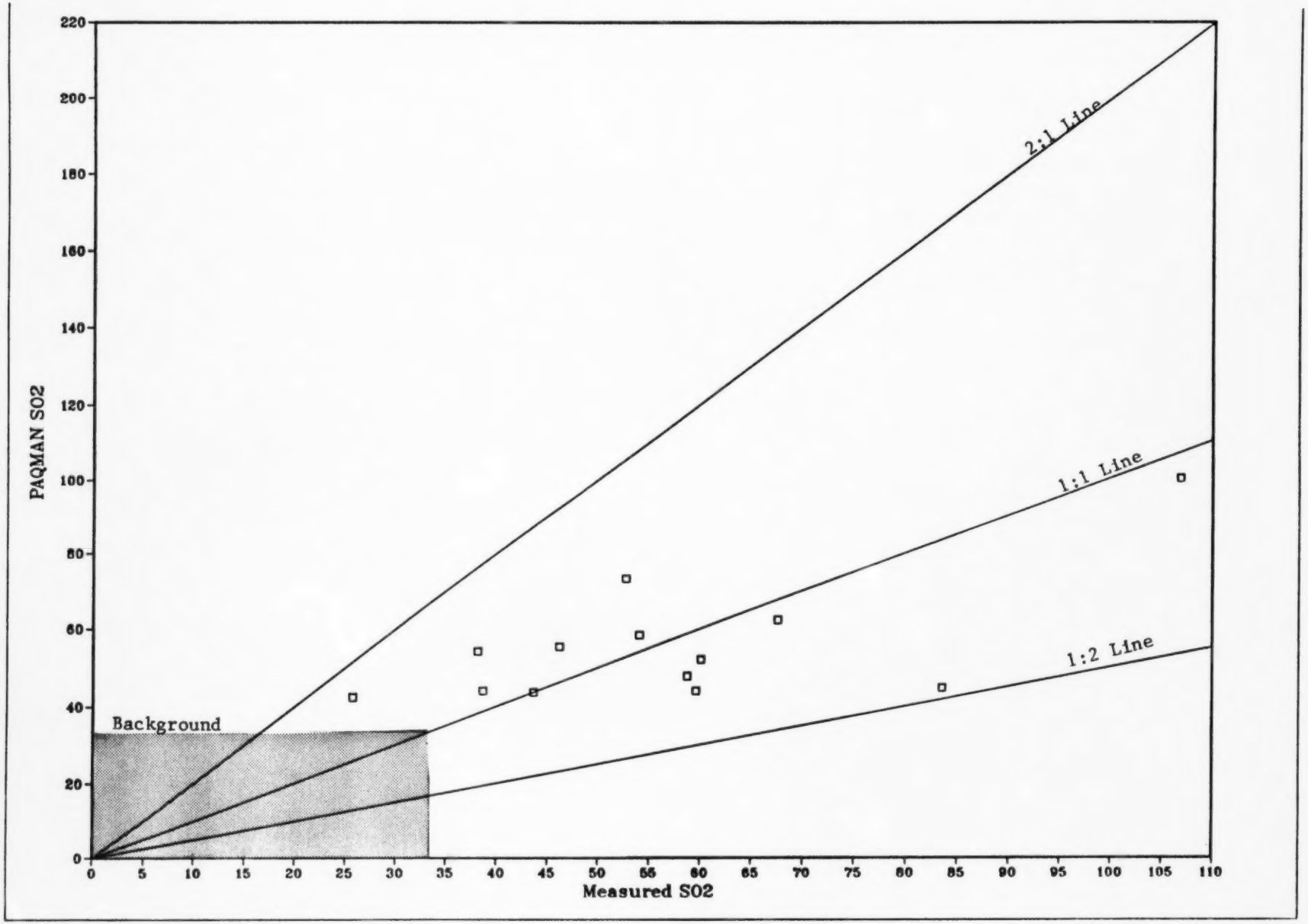


Figure 24. Comparison of PAQMAN vs. measured SO_2 - Pittsburgh, PA

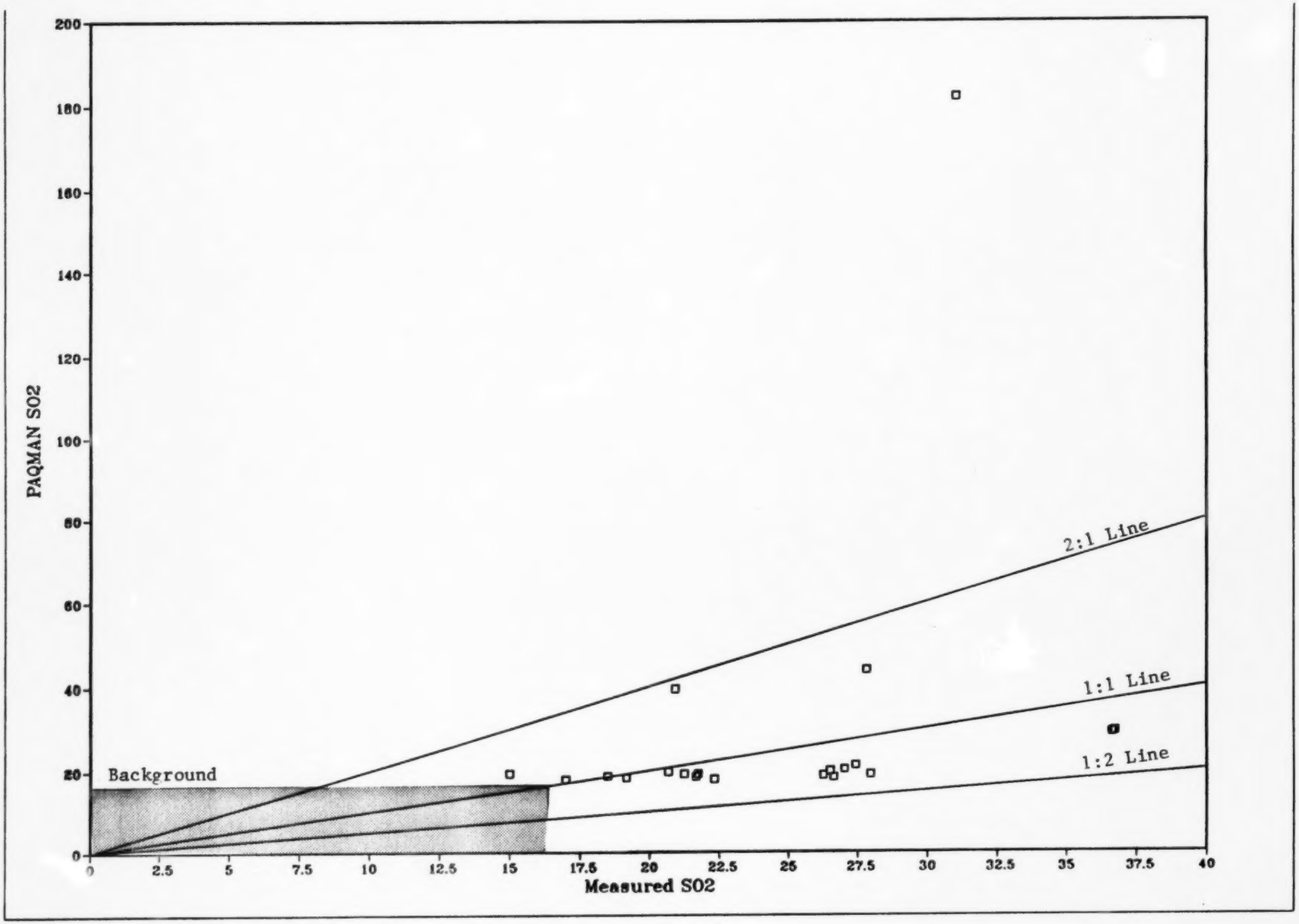


Figure 25. Comparison of PAQMAN vs. measured SO_2 - Washington, DC

Table 9. PAQMAN vs. Monitored Data Comparisons

City	PAQMAN MSA-Average*	Measured MSA-Average	PAQMAN/Measured Mean	Median	% ±2	% ±1.5	Slope of Linear Regression**
Baltimore	28.3	24.3	1.27	1.04	97	71	1.30
Boston	22.8	25.8	1.01	0.84	95	68	0.97
Chicago	38.0	24.4	1.55	1.26	87	62	1.52
Cincinnati	33.0	31.1	1.14	1.14	100	86	1.06
Cleveland	46.0	37.0	1.14	1.03	95	82	1.18
New York City	26.0	35.8	0.83	0.76	88	73	0.73
Philadelphia	34.7	36.7	1.10	1.02	97	76	1.01
Pittsburgh	55.5	57.6	1.05	0.97	100	85	0.93
Washington, DC	26.5	24.6	1.19	0.85	95	85	1.28
Average±	34.5	32.9	1.17	1.03	95	76	1.11

* Average for grid squares with monitored data (background included).
**Regression forced through origin. PAQMAN value as dependent variable.
± Average over entire data set.

centroids for Baltimore and Washington, respectively. Similarly, for Chicago, a group of over 30 individual stacks from 4 different sources fell within the same grid square at a range of 0.86 to 2.48 km from the grid square centroid. Aggregating the emissions from all of these sources in the area source mode produced a predicted concentration of 15 $\mu g/m^3$ (168 $\mu g/m^3$ including background), while treating the source individually as point sources would result in a prediction of 12 $\mu g/m^3$ (26 $\mu g/m^3$ with background added) at the grid centroid. It is possible that downwash effects could result in some very high concentrations in the vicinity of the stacks, but the effect would be quite localized. This again indicates that these isolated cases must be further investigated and perhaps should be treated separately.

Bearing in mind that the interest in terms of damage assessments is the aggregated effect across over many MSA's, the model performs reasonably well. In this context, overpredictions (relative to measured data) in some localities tend to be offset by underpredictions in others, as shown in Table 9.

4.0 CONCLUSIONS

A method of estimating annual average SO_2 concentration levels in urban areas has been developed, to be used in conjunction with damage functions to derive aggregate economic estimates of materials damage for large metropolitan areas. The modeling system, PAQMAN, consists of a set of simplified closed-form algorithms which mimic the performance of EPA's CDM model, and allows for the rapid assessment of a large number of sources and receptors. Earlier studies, in which the model was exercised for over 100 MSA's throughout the Northeastern U.S., indicated reasonable agreement between model predictions and observed values on an overall, aggregate basis. Further sensitivity analyses of various model components and assumptions were performed, and the results indicate that some improvements/modifications should be made to PAQMAN. These include:

1. The area source calculation scheme should be further examined. The model may be underpredicting area source impacts at the lower (ie. 1-2 km) emission grid scales.

2. The criterion used to estimate the effect of neighboring emission grids in the area source algorithms should be adjusted. The model appears to be underpredicting these impacts, particularly at the lower grid-scale levels where emission densities tend to be non-homogeneous from one cell to another.

3. The concept of defining a given source as a point or area source based on stack height does have some merit, but the impact of a given source, as predicted by PAQMAN, is very sensitive to its treatment as an area or a point source. While area source impacts are averaged over a grid square, point source effects are distance-dependent. Thus, the impacts of point sources may be underestimated in the model, particularly for larger grid sizes. A similar concept of averaging the point source impacts over a given area (as applied in the area source algorithms) may be more appropriate and should be investigated.

4. Depending on the orientation of major point sources with respect to a given MSA, PAQMAN over- or underpredicts point source impacts for some individual MSA's. (This is due to the directional-averaging procedure adapted in the parametric CDM modeling runs used to develop the point source algorithms.) Although the bias is found only for lower SO_2 levels, the results indicate that wind-direction effects should be accounted for.

5. The relationships found between stack height, maximum ground-level concentration and distance to the maximum concentration in the original parametric CDM studies using the McElroy-Pooler dispersion coefficients appear to be supported using Briggs' coefficients (rural values adjusted upwards by one stability class to account for increased dispersion in urban areas). However, the concept of collapsing all stack heights to a single representation needs to be examined further. Results using the Briggs' coefficients suggest that separate point source algorithms should be derived for shorter and taller stacks.

In spite of these areas of uncertainty, PAQMAN predictions compare with observed values (same grid square) generally within a factor of 2 for many of the larger city networks. Comparison of MSA-averaged predicted and observed values showed fair agreement (slope of 0.81), suggesting that individual source errors are smoothed out in the aggregate. This is even more apparent when the effects of individual MSA's are aggregated across an entire region such as the Northeast U.S.

In the context of aggregated effects across a large region involving thousands of individual sources, PAQMAN is a very useful and suitable tool for estimating SO_2 distributions in urban areas. Its automated source-receptor allocation procedures allow the rapid assessment of impacts for many sources and receptors, greatly reducing excessive user-input requirements as well as computer storage and running times. If the scope of the materials assessment narrows to a single-city analysis (or detailed analysis of a few cities), a more sophisticated model may be more suitable, but certainly some of the automated procedures developed in PAQMAN would be useful in other models as well and should be considered.

5.0. REFERENCES

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